A new approach to lattice quantum field theories

A THESIS
SUBMITTED TO THE FACULTY OF THE GRADUATE SCHOOL
OF THE UNIVERSITY OF MINNESOTA
BY

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IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE OF
MASTER OF SCIENCE

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January 2018

Acknowledgements

There are many people that have earned my gratitude for their contribution to my time in graduate school. First among them is my advisor Dr. Vitaly Vanchurin whose constant push made me work even harder, Dr. Yang Li with whom I enjoyed many fruitful discussions, all of my professors whom I took classes with and had the opportunity to learn from them. Last but not the least, my friends and fellow graduate students with whom I shared many unforgettable and cherished moments. I also wish to thank a fellow graduate student Ankit Gupta from Dept. of Computer Science who helped me deal with some last moment issues with LaTex.

Dedication

To my lovely family and friends who held me up over the years and never gave up on me.

Abstract

In this thesis report, I describe an algorithm for lattice simulation of quantum/statistical fields that reduces the complexity of current techniques (Metropolis algorithm) from exponential in all the directions of space and (Euclidean-)time, to linear in (Euclidean-)time and exponential in space. This is done by building a typical field configuration spatial slice by spatial slice through an analytically obtained Markov chain from its path integral. Although the complexity still depends exponentially on the number of spatial lattice points, for quantum mechanics ($0+1$ fields) spatial slice is only a point and thus the complexity only depends linearly on the number of time lattice points and simulation becomes pretty easy. As examples, I discuss the cases of harmonic and an-harmonic oscillators along with some simulation results. The case of Gaussian fields in general (in any dimension) is trivial since in the similarity transformed space each lattice site decouples and hence there exists a random variable at each lattice site that does not interact with any other. Although the reduction of complexity from exponential in space (if possible) for higher dimensional fields in general is currently under investigation, I present a checkerboard network that we investigated along with some simulation results.

Contents

1 Introduction

1.1 Lagrangian formalism of Classical Mechanics

Quest to understand Nature has been a long going effort, relics of which can be dated (so far) as far back as 200 BC when the ancient Greeks, Chinese and Indians began thinking of matter as made up of indestructible constituents and had also developed quite a handful of techniques of observational astronomy. It was not until late 16th century though, when Principia was published by Newton and paved the way for the now called Classical Physics, that it became widely accepted that Mathematics is the language one needs to describe Nature in a rational and logically consistent way. Quite some time later in 1788, came along an Italian-French mathematician and astronomer named Joseph-Louis Lagrange who introduced the Lagrangian formulation of Classical Mechanics and with the combined efforts of many, it has now become one of the fundamental branches of Physics. Without dwelling into the history much, let's consider for starters a simple example where we have a point particle[1] of mass m, free to move in 3-D space labeled by Cartesian coordinates x, y, z and subject to a potential $V(x,y,z)$. One then begins by writing down a quantity known as the 'Lagrangian' L for this system:

$$L = \frac{m}{2}\left(\frac{d\vec{x}}{dt}\right)^2 - V(x,y,z) \tag{1.1}$$

[1] Note that the notion of point particle is debatable and is a subject of great importance in modern Physics, specially in String theory. But for the purposes of illustration, it is not going to pose any kind of issue.

which is just $T-V$.[2] Lagrangians of this form are called 'canonical'. Then one defines an action functional S from time t_0 to t_n as:

$$S[x,y,z] \equiv \int_{t_0}^{t_n} d\,t\; L \tag{1.2}$$

and it is this action that one can treat as a fundamental quantity that contains all the physics of our system of a point particle. Next, to get the equation of motion for the particle, one varies the action functional w.r.t. paths $\vec{x}(t)$ keeping the end points $\vec{x}(t_0)$, $\vec{x}(t_n)$ fixed, and set the variation to zero. This is called the 'least action principle' which states that the classical trajectory followed by the particle (given boundary conditions) is the one for which the action is extremized.

$$\frac{\delta S}{\delta \vec{x}(t)} = \int_{t_0}^{t_n} dt \left[-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{x}}}\right) + \frac{\partial L}{\partial \vec{x}} \right] = 0 \tag{1.3}$$

where $\dot{x}$ is the time derivative. Since the variation must be zero for all intervals, the integrand must be zero and thus we have what are called the Euler-Lagrange's equation:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{x}}}\right) = \frac{\partial L}{\partial \vec{x}} \tag{1.4}$$

For canonical Lagrangians (1.1), one thus have the good old Newton's equation of motion

$$m\ddot{\vec{x}} = -\frac{\partial V}{\partial \vec{x}} \tag{1.5}$$

As an illustration, consider a one dimensional harmonic oscillator with $V(x) = kx^2/2$ where k is some constant (known as spring constant). The equation of motion is then the good old

[2] here T stands for kinetic energy and V for potential energy of the particle. Note that in general, it is *not* true that L is simply equal to $T-V$, but for our purposes it would be true with some redefinition of what is meant by kinetic energy for the case of fields.

Hooke's law:

$$m\ddot{x} = -kx, \tag{1.6}$$

the solutions of which are circular functions and in general one can write for the solution

$$x(t) = x_0 \sin(\omega t + \phi) \tag{1.7}$$

where x_0 and ϕ are determined by boundary conditions. With this, we have completely described the system and have predicted how the harmonic oscillator will behave in the future given enough initial data.[3] At this point, I would like to mention that there is another equivalent formulation of Classical Physics known as the Hamiltonian formulation[1–3] in which instead of having a Lagrangian, one has the so called Hamiltonian of a system, which however I am not going to talk much about it in this thesis report.

Now all this can be easily generalized to something called fields which are simply functions of both space and time, and the nature of the function depends on the physics it describes. For example, a temperature field is a real scalar field which is nothing but a real valued function of space and time. Then one can write down a Lagrangian for it and obtain classical equation of motion by setting the first variation of action with respect to field configurations equal to zero. Another classical example is that of an electromagnetic field which is a vector field. That is, it is a set of three fields (in three dimensional space) or three functions together forming a 3-vector. Similarly, there can be a tensor field, for example gravitational field is a rank 2 tensor field and many more[4]. To build an intuition for a field, say a real scalar field, one may consider discretized space and at each lattice site $\vec{x}$, assign a 'position' function (a function of time) $\varphi^{\vec{x}}(t)$. That is, at each lattice site

[3] In general there are other quantities that are of interest, namely the energy of the system, it's angular momentum etc. which are all well understood quantities.

[4] Of particular interest are spinor fields which describe the physics of fermions[4–6].

we have the usual classical mechanical 'particle' and the whole system is then a many-'particle' system. The continuous field is then understood in the limit as discretization goes to zero and space becomes continuous. For instance, consider a scalar field $\varphi(\vec{x},t)$[5] defined within a box of volume V. In the discretized space limit, the Lagrangian, along the lines of many 'particle' system, can be written as

$$L = \varepsilon^D \sum_{\vec{x}}^{\vec{N}_s} \left(\left(\frac{d\varphi^{\vec{x}}}{dt} \right)^2 - V' \left(\varphi^{\vec{x}+\vec{\varepsilon}}, \varphi^{\vec{x}} \right) \right) \tag{1.8}$$

where $\vec{x}$ is the vector index spanning each direction in the D-dimensional spatial volume lattice, ε and N_s are the the discretization step and total number of lattice points in each direction respectively, and V' is a potential function which usually contains local interactions between different $\varphi^{\vec{x}}$'s along with some self interactions:

$$\begin{aligned} V' \left(\varphi^{\vec{x}+\vec{\varepsilon}}, \varphi^{\vec{x}} \right) &= \sum_{i=1}^{D} \left(\frac{\varphi^{x^i+\varepsilon} - \varphi^{x^i}}{\varepsilon} \right)^2 + V \left(\varphi^{\vec{x}} \right) \\ &\equiv \left(\frac{\varphi^{\vec{x}+\vec{\varepsilon}} - \varphi^{\vec{x}}}{\varepsilon} \right)^2 + V \left(\varphi^{\vec{x}} \right) \end{aligned} \tag{1.9}$$

where V is some self interaction potential function, i spans all directions in spatial lattice, and in the last line I've defined a notation for all nearby interactions. In the continuum limit where $\vec{x}$ becomes a continuous index and each i^{th} direction of space is labeled by a real number x^i, the Lagrangian becomes

$$\begin{aligned} L &= \int_{\mathcal{V}} d\mathcal{V} \left(\left(\frac{\partial \varphi(\vec{x},t)}{\partial t} \right)^2 - \left(\frac{\partial \varphi(\vec{x},t)}{\partial x^1} \right)^2 - \left(\frac{\partial \varphi(\vec{x},t)}{\partial x^2} \right)^2 - \ldots - V\left(\varphi(\vec{x},t)\right) \right) \\ &\equiv \int_{\mathcal{V}} d\mathcal{V} \mathcal{L} \left(\varphi, \partial_\mu \varphi \right) \end{aligned} \tag{1.10}$$

[5] note that I write superscripts to denote the fact that I'm working in discrete space limit, and arguments to denote a continuous space

where $\mathcal{V}$ is spatial volume, $\mathcal{L}$ is called the Lagrangian density, the index μ spans the space-time coordinates[6], and $\partial_\mu\varphi$ denotes partial derivative w.r.t. μth coordinate ($\partial_\mu \equiv \partial/\partial x^\mu$). We therefore have the following action

$$S[\varphi(x^\mu)] \equiv \int_{t_0}^{t_n} dt \int_V dV \, \mathcal{L}\left(\varphi, \partial_\mu\varphi\right) \tag{1.11}$$

with the following classical equation of motion

$$\partial_\mu \left(\frac{\partial L}{\partial\left(\partial_\mu\varphi\right)} \right) = \frac{\partial L}{\partial\varphi} \tag{1.12}$$

obtained by setting first variation of S w.r.t. $\varphi(x^\mu)$ equal to zero and keeping the boundary configurations fixed. As an illustration, consider a a real scalar field in $3+1$ dimensions (with time denoted by t and spatial directions by x, y, z) with the following canonical Lagrangian density

$$\mathcal{L} = \frac{1}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\varphi}{\partial x}\right)^2 - \frac{1}{2}\left(\frac{\partial\varphi}{\partial y}\right)^2 - \frac{1}{2}\left(\frac{\partial\varphi}{\partial z}\right)^2 - V(\varphi) \tag{1.13}$$

The equation of motion obtained from least action principle is

$$\Box\varphi + \frac{\partial V}{\partial\varphi} = 0 \tag{1.14}$$

where $\Box$ is called the D' Alembertian or the Box operator:

$$\Box \equiv \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2. \tag{1.15}$$

A well known example (which will be of central physical importance to us) is that of a

[6] in the convention I'm using, I take $x^0 = t$, and rest indices are for spatial directions. Usually we are interested in 3 dimensional space (along with one direction of time) and thus μ goes from 0 to 3.

Klein-Gordan field[4–6] with $V(\varphi) = \frac{1}{2}m^2\varphi^2$ where m is called the mass of the field. The equation of motion is then

$$\left(\Box + m^2\right)\varphi = 0 \tag{1.16}$$

So much for the classical description of particles and fields. Although there is a whole career one can make in just the classical study of interesting systems, Nature in its purest and deepest form seems to behave rather strangely in a way in which all of our classical intuition just gets thrown out of the window. This strangeness (studied under the name of quantum physics) is apparent and dominating at small enough scales and one cannot avoid describing the physics of a system correctly without describing its quantum mechanical behavior. At large enough scales (the scales that we humans deal with in our usual lives), classical point of view emerges and the effective description can be pretty accurately approximated by the good old classical mechanics.

1.2 Transition to the quantum world in the Lagrangian formalism

Although there are 2 well known different but equivalent formulations of Quantum Mechanics, I will present the so called Lagrangian formulation or path integral formulation discovered by Richard P. Feynman[7–9].[7]To begin with, in the quantum mechanical description, state of the system is not characterized by its position and velocity (more generally momentum) as in classical mechanics, but by something called the *wave function* Ψ which is a complex function of spatial coordinates (or momenta) and time. Then the proba-

[7]The other description is called the Dirac or canonical quantization[4–6][10–15] that begins with Hamiltonian formulation of classical physics, developed fully by Paul Dirac, with notable contributions from a number of Physicists and is tied intimately with the Lagrangian formulation. There is yet another formulation called the phase space formulation[16–19] of Quantum Mechanics and is quite different from the former two formulations.

bility distribution ρ for position (or momenta) as a function of time is given by the absolute square of this wave function ($\rho = \Psi^*\Psi$), meaning that there exists a probability distribution for the positions (or momenta) of the system rather than specific values.[8] Again as before, various measurable quantities like energy, angular momentum etc. are well understood in quantum physics.[9] Anyways, the time evolution of the wave function is governed by the Kernel K of Schrdinger's equation[10] according to the following:

$$\psi(\vec{x_N}, t_N) = \int d^3x_0 K(\vec{x}_N, t_N; \vec{x}_0, t_0)\, \psi(\vec{x}_0, t_0) \tag{1.17}$$

Here, the kernel is said to propagate the wave function from time t_0 to t_N. In the canonical quantization formalism, this is equivalent to the evolution of the state $|\psi\rangle$ (which is a vector in a Hilbert space) by a unitary operator $U(t_{t_N}, t_0)$[4–6][10–15]:

$$|\psi\rangle_{t_N} = U(t_{t_N}, t_0)|\psi\rangle_{t_0} \tag{1.18}$$

Now from the Lagrangian formulation point of view, the kernel, also known as the *probability amplitude* for the system to go from initial configuration $\vec{x}_0$ at t_0 to final configuration $\vec{x}_N$ at t_N is given by the sum of *all* possible paths weighted by the functional $e^{iS/\hbar}$ where $\hbar$ is the Planck's constant. That is

$$K(\vec{x}_N, t_N; \vec{x}_0, t_0) = \int_{\vec{x}_0}^{\vec{x}_N} D[\vec{x}] e^{\frac{i}{\hbar} S_{t_0 \to t_N}} \tag{1.19}$$

Here, the integration measure is understood as integration over all possible paths/functions $x(t)$ with end points fixed at x_0 and x_N at time t_0 and t_N respectively. Note that the weight

[8] The very notion of specific positions/momenta of a system does not exist because of wave particle duality. For more, see[13–15].

[9] These quantities can only form a discrete spectrum and at large scales, they appear to be forming a continuous spectrum as dictated by the laws of classical mechanics.

[10] for a detailed discussion, see canonical quantization[4–6][10–15]

functional is a complex number and therefore the kernel function is a complex valued function. Now to address the issue of integration over all possible paths, there are a handful of techniques physicists have developed. Since the end points are fixed for any path, we can decompose it in a Fourier series and then have all possible paths by allowing all possible Fourier coefficients. Thus, integration over all possible paths can be understood as integration over all possible Fourier coefficients. Another way is to discretize the integration variable(s) in the action, making any path piece-wise with say N intermediate points, and the action then is a function of these N intermediate path points and the two boundary points. Then, integration over all these intermediate path points suffices and integration over all possible paths is understood as a limit when the discretization step goes to zero and number of intermediate steps goes to infinity keeping the product (i.e. the total integration interval in the action) fixed. It is this discretization approach that I would be making use of in all of my work. Consider time discretization with ε as the time step such that

$$\varepsilon = \frac{t_N - t_0}{N-1}, \qquad \text{and} \tag{1.20}$$

and therefore

$$S(\{\vec{x}_k\}) = \varepsilon \sum_{i=0}^{N-1} L\left(\frac{\vec{x}_{i+1}-\vec{x}_i}{\varepsilon}, \frac{\vec{x}_{i+1}+\vec{x}_i}{2}\right) \equiv \sum_{i=0}^{N-1} S_d(\vec{x}_{i+1}, \vec{x}_i) \tag{1.21}$$

where $(\vec{x}_{k+1}-\vec{x}_k)/\varepsilon$, and $(\vec{x}_{k+1}+\vec{x}_k)/2$ denote $\dot{\vec{x}}$ and $\vec{x}$ at the kth time step in the discrete limit. Then, the kernel is given by

$$K(\vec{x}_N, t_N; \vec{x}_0, t_0) = \prod_{j=1}^{N-1} \int_{-\infty}^{\infty} \frac{d^3x_j}{\sqrt{2\pi\varepsilon/\hbar}} e^{\frac{i}{\hbar}S(\{x_k\})}. \tag{1.22}$$

This is the discretized version understood properly as integration over many variables. At this point I would like to point out the following fact

$$K\left(\vec{x},t'';\vec{y},t\right)=\int d^3z\,K\left(\vec{x},t'';\vec{z},t'\right)K\left(\vec{z},t';\vec{y},t\right) \tag{1.23}$$

where $t''>t'>t$ and can be easily seen from the evolution equation (1.17). Therefore for just one time step, we have

$$\psi\left(\vec{x}_{k+1},t_{k+1}\right)=\int d^3x_k K\left(\vec{x}_{k+1},t_{k+1};\vec{x}_k,t_k\right)\psi\left(\vec{x}_k,t_k\right) \tag{1.24}$$

where

$$K\left(\vec{x}_{k+1},t_{k+1};\vec{x}_k,t_k\right)=\sqrt{\frac{\hbar}{2\pi\varepsilon}}e^{\frac{i}{\hbar}S_d\left(\vec{x}_{k+1},\vec{x}_k\right)}. \tag{1.25}$$

Now, all the eigenstates of this kernel form a spectrum known as the energy eigen spectrum and are separable functions of time and space:

$$\begin{aligned}\psi_n\left(\vec{x}_{k+1}\right)e^{\frac{i}{\hbar}E_n t_{k+1}} &= \int d^3x_k K\left(\vec{x}_{k+1},t_{k+1};\vec{x}_k,t_k\right)\psi\left(\vec{x}_k\right)e^{\frac{i}{\hbar}E_n t_k}\\ \implies e^{\frac{i}{\hbar}\varepsilon E_n}\psi_n\left(\vec{x}_{k+1}\right) &= \int d^3x_k K\left(\vec{x}_{k+1},t_{k+1};\vec{x}_k,t_k\right)\psi_n\left(\vec{x}_k\right)\end{aligned} \tag{1.26}$$

Here, n spans the ordered eigenvalue set (spectrum) and the time-independent parts are called nth energy states (with energy E_n), with the 'ground' state being the one with $n=0$ (i.e. with the smallest energy value) and denoted by $|0\rangle$.[11] Usually in quantum mechanics, one is interested in finding the probability of finding the system in some state $|\phi\rangle$ at time t_N given initially in state $|\Psi\rangle$ at t_0. This is given by the projection (inner product) of the evolved initial state (wave function) up to time t_N onto ϕ at t_N, with the evolution operator

[11] In the canonical formalism, it is the Hamiltonian operator H whose eigenstates are the same as kernel's, but with the eigenvalues being E_n instead of $e^{\frac{i}{\hbar}\varepsilon E_n}$ and are obviously time independent, hence the terminology.

$U(t_N,t_0)$:

$$\langle\phi|U(t_N,t_0)|\Psi\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3x_0 d^3x_N \phi^*(\vec{x_N},t_N)\, K\left(\vec{x}_N,t_N;\vec{x}_0,t_0\right)\psi(\vec{x}_0,t_0) \tag{1.27}$$

and squaring it, i.e. the probability of transition to $|\phi\rangle$ at t_N from $|\psi\rangle$ at t_0. With all this, transition from ground state at t_0 to ground state at t_N is therefore

$$\begin{aligned}
\langle 0|U(t_N,t_0)|0\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3x_0 d^3x_N \psi_0^*(\vec{x_N})\, K\left(\vec{x}_N,t_N;\vec{x}_0,t_0\right)\psi_0(\vec{x}_0) \\
&= \prod_{i=0}^{N}\int_{-\infty}^{\infty} d^3x_i\, \psi_0^*(\vec{x_N})\, K\left(\vec{x}_N,t_N;\vec{x}_{N-1},t_{N-1}\right)...K\left(\vec{x}_1,t_1;\vec{x}_0,t_0\right)\psi_0(\vec{x}_0) \\
&= e^{\frac{i}{\hbar}E_0(t_N-t_0)}
\end{aligned} \tag{1.28}$$

We can redefine the kernel by absorbing the ground state eigenvalue $e^{\frac{i}{\hbar}\varepsilon E_0}$:

$$\tilde{K}\left(\vec{x}_k,t_k;\vec{x}_{k-1},t_{k-1}\right) \equiv K\left(\vec{x}_k,t_k;\vec{x}_{k-1},t_{k-1}\right) e^{-\frac{i}{\hbar}\varepsilon E_0} \tag{1.29}$$

and therefore have

$$\begin{aligned}
\langle 0|\tilde{U}(t_N,t_0)|0\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3x_0 d^3x_N \psi_0^*(\vec{x_N})\, \tilde{K}\left(\vec{x}_N,t_N;\vec{x}_0,t_0\right)\psi_0(\vec{x}_0) \\
&= \prod_{i=1}^{N-1}\int_{-\infty}^{\infty} d^3x_i\, \psi_0^*(\vec{x_N})\, \tilde{K}\left(\vec{x}_N,t_N;\vec{x}_{N-1},t_{N-1}\right)...\tilde{K}\left(\vec{x}_1,t_1;\vec{x}_0,t_0\right)\psi_0(\vec{x}_0) \\
&= 1
\end{aligned} \tag{1.30}$$

Note that this is tantamount to adding a constant term $= -E_0$ in the Lagrangian, i.e. just shifting the potential by E_0 [12]. In general, we are interested in the n-point correlation

[12] Although it is of no significance to us, this is known as the cosmological constant term in the Lagrangian and becomes important when there is also gravity.

functions. Before defining them, consider the following object

$$
\begin{aligned}
& G(t_k) \equiv \frac{\langle 0|U(t_N,t_{k+1})\vec{x}_k U(t_{k-1},t_0)|0\rangle}{\langle 0|U(t_N,t_0)|0\rangle} \\
= & \frac{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3x_0\, d^3x_{k-1}\, d^3x_{k+1}\psi_0^*(\vec{x_N})\, K\left(\vec{x}_N,t_N;\vec{x}_{k+1},t_{k+1}\right)\vec{x}_k\, K\left(\vec{x}_{k-1},t_{k-1};\vec{x}_0,t_0\right)\psi_0(\vec{x}_0)}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3x_0 d^3x_N \psi_0^*(\vec{x_N})\, K\left(\vec{x}_N,t_N;\vec{x}_0,t_0\right)\psi_0(\vec{x}_0)} \\
= & \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^3x_0\, d^3x_{k-1}\, d^3x_{k+1}\psi_0^*(\vec{x_N})\, \tilde{K}\left(\vec{x}_N,t_N;\vec{x}_{k+1},t_{k+1}\right)\vec{x}_k\, \tilde{K}\left(\vec{x}_{k-1},t_{k-1};\vec{x}_0,t_0\right)\psi_0(\vec{x}_0) \\
= & \langle 0|\tilde{U}(t_N,t_{k+1})\vec{x}_k\tilde{U}(t_{k-1},t_0)|0\rangle \qquad (1.31)
\end{aligned}
$$

where off course $t_N > t_k > t_0$. This is called 1-point correlation function simply because it is the average of $\vec{x}$ at t_k over the ground state fluctuations (within time period $t_N - t_0$). Similarly, any n-point correlation function, call it $G_n(\vec{x}_n,...,\vec{x}_1)$ is given by

$$
\begin{aligned}
G_n(\vec{x}_n,...,\vec{x}_1) &= \frac{\langle 0|U(t_N,t_n)\vec{x}_n U(t_n,t_{n-1})\vec{x}_{n-1}...U(t_2,t_1)\vec{x}_1 U(t_1,t_0)|0\rangle}{\langle 0|U(t_N,t_0)|0\rangle} \\
&= \langle 0|\tilde{U}(t_N,t_n)\vec{x}_n\tilde{U}(t_n,t_{n-1})\vec{x}_{n-1}...\tilde{U}(t_2,t_1)\vec{x}_1\tilde{U}(t_1,t_0)|0\rangle \qquad (1.32)
\end{aligned}
$$

where it must be understood that $t_N > t_n > ... > t_1 > t_0$ and all insertions of $\vec{x}$'s are made similarly as in the above expression i.e. there is a kernel in between every adjacent pair of $\vec{x}$'s and integration over all intermediate points is to be done.

Moving on, this whole formalism can be generalized to fields which in the discretized space limit, is just the extension of the discussion so far with many 'particles'[13]. Consider a real scalar field $\varphi(\vec{x},t)$ in $3+1$ dimensions with the Lagrangian density (1.13). The kernel

[13]The reason I've been writing quotes around particles is that particles have a well understood meaning, specially in the case of Quantum fields. A Fourier excitation of the field is thought of as a particle state with its momentum depending upon the value of the excited Fourier mode. I am unable to think of a good name for the lattice sites and still want to emphasize that these are not *the* particles of a quantum field theory, hence the quotes

(in the discrete space limit) is given by

$$K\left(\vec{\varphi},t_N;\vec{\varphi},t_0\right)=\prod_{j=1}^{N-1}\int_{\vec{\varphi}(t_0)}^{\vec{\varphi}(t_N)}D[\vec{\varphi}_j]e^{\frac{i}{\hbar}S_{t_N\to t_0}} \tag{1.33}$$

where the index j spans time steps (total time steps being equal to N), vector notation for φ's is to be understood in the sense that the vector label would span all the spatial lattice sites[14] (also equal to N_s) and therefore each measure $D[\vec{\varphi}_j]$ is a product of the measures like (1.19) for each lattice site. Off-course $\vec{\varphi}(t_0)$ and $\vec{\varphi}(t_N)$ are the initial and final field configurations at t_0 and t_N respectively. The many 'particle' action (discretized) is given by (c.f. (1.8))

$$S_{t_N\to t_0}=\varepsilon\varepsilon^3\sum_{j=0}^{N}\sum_{\vec{x}=\vec{0}}^{\vec{N}_s}\left[\left(\frac{\varphi_{j+1}^{\vec{x}}-\varphi_j^{\vec{x}}}{\varepsilon}\right)^2-\left(\frac{\varphi_j^{\vec{x}+\vec{\varepsilon}}-\varphi_j^{\vec{x}}}{\varepsilon}\right)^2-V\left(\varphi_j^{\vec{x}}\right)\right]\equiv\sum_{j=0}^{N}S_d(\vec{\varphi}_{j+1},\vec{\varphi}_j) \tag{1.34}$$

where ε is the discretization step in time (equal to that of each spatial direction), $\vec{x}$ spans all spatial lattice sites as before, and j spans time steps. The first bracket denotes connection in time, and the second bracket is a sum of three such brackets denoting similar (space) connections in each spatial direction (c.f. (1.9)). Note that time and space are on equal footing as both the time and space discretization are equal. With this, time evolution of our many 'particle' wave-function is given as

$$\psi(\vec{\varphi},t)=\int D[\vec{\varphi}']K\left(\vec{\varphi},t;\vec{\varphi}',t'\right)\psi(\vec{\varphi}',t') \tag{1.35}$$

with off course $t>t'$. Also for just one time step, we have (similarly as before)

$$K\left(\vec{\varphi}_{k+1},t_{k+1};\vec{\varphi}_k,t_k\right)=\left(\sqrt{\frac{\hbar}{2\pi\varepsilon\delta V}}\right)^{N_s}e^{\frac{i}{\hbar}S_d(\vec{\varphi}_{i+1},\vec{\varphi}_i)}. \tag{1.36}$$

[14] superscript spanning lattice sites are now denoted in a vector notation i.e. $\varphi^{\vec{x}}$'s $\to\vec{\varphi}$

The ground state to ground state transition then (as before) is given by

$$\begin{aligned}\langle 0|\tilde{U}(t_N,t_0)|0\rangle &= \int\int D[\vec{\varphi}_N]D[\vec{\varphi}_0]\psi_0^*(\vec{\varphi}_N)\,\tilde{K}\,(\vec{\varphi}_N,t_N;\vec{\varphi}_0,t_0)\,\psi_0(\vec{\varphi}_0)\\ &= \prod_{i=1}^{N-1}\int D\vec{\varphi}_i\,\psi_0^*(\vec{\varphi}_N)\,\tilde{K}\,(\vec{\varphi}_N,t_N;\vec{\varphi}_{N-1},t_{N-1})\ldots\tilde{K}\,(\vec{\varphi}_1,t_1;\vec{\varphi}_0,t_0)\,\psi_0(\vec{\varphi}_0)\\ &= 1 \end{aligned} \tag{1.37}$$

As before, I have absorbed the ground state eigenvalue in redefining the kernel. Finally, any n point correlation function is given by

$$G(\vec{x}_n,\ldots,\vec{x}_1) = \langle 0|\tilde{U}(t_N,t_n)\vec{\varphi}_n\tilde{U}(t_n,t_{n-1})\vec{\varphi}_{n-1}\ldots\tilde{U}(t_2,t_1)\vec{\varphi}_1\tilde{U}(t_1,t_0)|0\rangle \tag{1.38}$$

with insertions made as described before and $t_N > t_n \ldots > t_0$. Now with all this, note that the kernel has oscillatory weight function ($e^{i\frac{S}{\hbar}}$) in the integrand and therefore the convergence of integral is a little obscure. To facilitate this point, one analytically continues the integrand in the complex space to make it real valued such that the integration can be performed and finally analytically continue it back to get the required answer[15]. I briefly address this in the next section.

1.2.1 Analytic continuation: from Minkowski to Euclidean metric

To understand analytical continuation, it's sufficient to consider just one time step. The integrand in K is the exponential of the action functional between two nearby spatial slices (c.f. (1.34)):

$$S_d\left(\vec{\varphi}_{j+1},\vec{\varphi}_j\right) = \varepsilon\varepsilon^3\sum_{\vec{x}=\vec{0}}^{\vec{N}}\left[\left(\frac{\varphi_{j+1}^{\vec{x}}-\varphi_j^{\vec{x}}}{\varepsilon}\right)^2 - \left(\frac{\varphi_j^{\vec{x}+\vec{\varepsilon}}-\varphi_j^{\vec{x}}}{\varepsilon}\right)^2 - V\left(\varphi_j^{\vec{x}}\right)\right]. \tag{1.39}$$

[15] Although analytical continuation may not be justified in general for any Lagrangian/action, for canonical Lagrangians/actions and therefore for our purposes, it is[4–6][20].

Then, we can analytically continue time in to the complex space $t \to \tau e^{-i\delta}$. In particular we consider analytical continuation where $\delta = \pi/2$, called 'Wick rotation' i.e. $t \to -i\tau$, or, for just one time step $\varepsilon \to -i\varepsilon$ and have

$$S_E\left(\vec{\varphi}_{j+1}, \vec{\varphi}_j\right) = i\varepsilon\varepsilon^3 \sum_{\vec{x}=\vec{0}}^{\vec{N}} \left[\left(\frac{\varphi_{j+1}^{\vec{x}} - \varphi_j^{\vec{x}}}{\varepsilon} \right)^2 + \left(\frac{\varphi_j^{\vec{x}+\vec{\varepsilon}} - \varphi_j^{\vec{x}}}{\varepsilon} \right)^2 + V\left(\varphi_j^{\vec{x}}\right) \right] \tag{1.40}$$

where E stands for 'Euclidean'[16]and I've dropped the subscript d with the hope that it is understood. The kernel for this time step then becomes (is analytically continued to)

$$K_E\left(\vec{\varphi}_{j+1}, \tau_{j+1}; \vec{\varphi}_j, \tau_j\right) = \left(\sqrt{\frac{\hbar}{2\pi\varepsilon}} \right)^{N_s} e^{-\frac{1}{\hbar} S_E} \tag{1.41}$$

and the eigenfunction equation becomes

$$e^{-\frac{\varepsilon}{\hbar} E_n} \psi_n\left(\vec{\varphi}_{j+1}\right) = \int D[\vec{\varphi}_j] K\left(\vec{\varphi}_{j+1}, \tau_{j+1}; \vec{\varphi}_j, \tau_j\right) \psi_n\left(\vec{\varphi}_j\right) \tag{1.42}$$

Note carefully the exponential suppression here. The ground state to ground state transition from Euclidean time τ_0 to τ_N would then be

$$\begin{aligned} \langle 0|U_E(\tau_N, \tau_0)|0\rangle &= \int\int D[\vec{\varphi}_0] D[\vec{\varphi}_N] \psi_0(\vec{\varphi}_N) K_E\left(\vec{\varphi}_N, \tau_N; \vec{\varphi}_0, \tau_0\right) \psi_0(\vec{\varphi}_0) \\ &= \prod_{i=0}^{N} \int D[\vec{\varphi}_i] \psi_0(\vec{\varphi}_N) K\left(\vec{\varphi}_N, \tau_N; \vec{\varphi}_{N-1}, \tau_{N-1}\right) \ldots K\left(\vec{\varphi}_1, \tau_1; \vec{\varphi}_0, \tau_0\right) \psi_0(\vec{\varphi}_0) \\ &= e^{-\frac{E_0}{\hbar}(\tau_N - \tau_0)} \end{aligned} \tag{1.43}$$

[16]The reason it is called Euclidean is obviously because the distance metric in the Wick rotated space is Euclidean.

where U_E is the Wick rotated operator. Similarly as before, I redefine the kernel by absorbing the ground state eigenvalue:

$$\tilde{K}_E\left(\vec{\varphi}_k,\tau_k;\vec{\varphi}_{k-1},\tau_{k-1}\right) \equiv K_E\left(\vec{\varphi}_k,\tau_k;\vec{\varphi}_{k-1},\tau_{k-1}\right) e^{-\frac{\varepsilon}{\hbar}E_0} \tag{1.44}$$

making the ground to ground state transition equal to unity:

$$\begin{aligned}
\langle 0|\tilde{U}(\tau_N,\tau_0)|0\rangle &= \int\int D[\vec{\varphi}_0]D[\vec{\varphi}_N]\psi_0(\vec{\varphi}_N)\,\tilde{K}_E\left(\vec{\varphi}_N,\tau_N;\vec{\varphi}_0,\tau_0\right)\psi_0(\vec{\varphi}_0) \\
&= \prod_{i=0}^{N}\int D[\vec{\varphi}_i]\psi_0(\vec{\varphi}_N)\,\tilde{K}_E\left(\vec{\varphi}_N,\tau_N;\vec{\varphi}_{N-1},\tau_{N-1}\right)...\tilde{K}_E\left(\vec{\varphi}_1,\tau_1;\vec{\varphi}_0,\tau_0\right)\psi_0(\vec{\varphi}_0) \\
&\equiv \prod_{i=0}^{N}\int D[\vec{\varphi}_i]\;\; P(\vec{\varphi}_N,\vec{\varphi}_{N-1},...,\vec{\varphi}_0) \\
&= 1
\end{aligned} \tag{1.45}$$

where I have now defined the probability distribution function (functional in the continuous space limit) for the field configuration (ground to ground state transition off-course). It should be noted that no matter what state we start with in the beginning at τ_0 (can be any linear combination of the eigenstates (energy eigenstates) of the kernel), successive application of the kernel (evolution of the state) will always result in the dominant/ground state because of the exponential suppression for all other states, the leading one (first excited state) being suppressed by $exp^{-(E_1-E_0)(\tau_N-\tau_0)}$ and so on[17]. Therefore we are guaranteed ground to ground transition in the long run (enough Euclidean time steps). Furthermore, it would also not matter what state is at the end of the transition (at τ_N) in the long run since in the bulk we are guaranteed ground to ground transition and what is at the end would only create a difference at the last time step which is only a boundary effect. Therefore,

[17] In general the suppression of a n^{th} excited state is

$$exp^{-(E_n-E_0)(\tau_N-\tau_0)}$$

any state to any state transition in the large bulk limit ($\tau_0 \to -\infty$ and $\tau_N \to \infty$) would be proportional to ground to ground state transition:

$$\lim_{\substack{\tau_0 \to -\infty \\ \tau_N \to \infty}} \langle f|\tilde{U}(\tau_N, \tau_0)|i\rangle \propto \langle 0|\tilde{U}(\infty, -\infty)|0\rangle \tag{1.46}$$

$$\propto \lim_{n\to\infty} \prod_{i=-n}^{n} \int D[\vec{\varphi}_i] \; P(\vec{\varphi}_n, \vec{\varphi}_{n-1}, ..., \vec{\varphi}_{-n-1}\vec{\varphi}_{-n}) \tag{1.47}$$

Because of the fact that the boundary states don't matter in the large bulk limit, one can simply drop ψ's from the probability distribution function definition and instead have

$$\lim_{n\to\infty} P(\vec{\varphi}_n, \vec{\varphi}_{n-1}, ..., \vec{\varphi}_{-n-1}\vec{\varphi}_{-n}) \propto \tilde{K}_E\left(\vec{\varphi}_n, \tau_n; \vec{\varphi}_{n-1}, \tau_{n-1}\right) ... \tilde{K}_E\left(\vec{\varphi}_{-n+1}, \tau_{-n+1}; \vec{\varphi}_{-n}, \tau_{-n}\right)$$

$$\propto e^{-\frac{1}{\hbar} S_E} \tag{1.48}$$

where the proportionality constant would depend on the boundary states. Finally, if one is able to simulate this field successfully (pick field configurations according to P and build enough sample space), useful statistics can be done. For example, any n-point correlator $\langle 0|\varphi(x_n)..\varphi(x_1)|0\rangle$ can be obtained as

$$G_n\left(x_n, ..., x_1\right) = \frac{1}{M} \sum_{i=1}^{M} \{\varphi(x_n)...\varphi(x_1)\}_i \tag{1.49}$$

where the index spans the sample space (of size M) and the argument x stands for all directions, including the 'Euclidean' time[18].

[18]From now on I'll denote the Euclidean time by t and stop writing Euclidean, and skip writing 0's to denote ground state, with the hope that these are understood

1.3 Mathematical statement of the Problem

Now that I have described in brief what the physics behind all my work is, here I pose the Mathematical problem we want to address in this thesis report:

Given a local probability distribution $P[\varphi]$ [19]for a random $D+1$ dimensional function $\varphi(x)$ (many random variables in the discretized version), we want to generate typical $D+1$-dimensional function realization(s) *from D dimensional slices* to obtain statistics (calculate various correlators) of it[20].

What I mean by local is that the action only contain a finite number of derivative couplings and no non-local couplings (usually for quantum fields, these are only second derivative couplings) apart from any self couplings. Also if there is translational ($\vec{x} \to \vec{x} + \vec{\alpha}$) and rotational symmetry ($\vec{x} \to R\vec{x}$) in P, only a single field (large enough) typical field configuration is enough to do all statistics. Specifically, the probability functionals that I am interested in are of the form

$$P[\varphi] \propto \exp\left(-S[\varphi]\right) \tag{1.50}$$

where

$$S[\varphi] = \int d^D x \left[\frac{1}{2}(\partial\varphi)^2 + V(\varphi)\right] \tag{1.51}$$

Here $V(\varphi)$ is some concave up function of φ and

$$(\partial\varphi)^2 \equiv \left(\frac{\partial\varphi}{\partial t}\right)^2 + \left(\frac{\partial\varphi}{\partial x}\right)^2 + \left(\frac{\partial\varphi}{\partial y}\right)^2 + \left(\frac{\partial\varphi}{\partial z}\right)^2 + \ldots \tag{1.52}$$

[19]I use square brackets to denote functionals as opposed to round brackets which are used to denote functions

[20]Note that if the distribution functional has certain properties such as rotational and translational symmetry in the x space which are my target functionals, only a single, large enough typical function configuration is enough in order to obtain correlators.

where the dots represents sum of the squares of partial derivatives w.r.t. all other directions of space (usually none). Once we have a typical function simulated on a discretized lattice, we can obtain all the n-point correlators by averaging over this field configuration. As an example, any two point correlator $G_2(\vec{x}_2,\vec{x}_1)$ can be obtained as

$$G_2(\vec{x}_2,\vec{x}_1) = \langle \varphi(\vec{x}_1)\varphi(\vec{x}_2)\rangle = \frac{1}{2n}\sum_i\sum_j \varphi(\vec{x}_i)\varphi(\vec{x}_j)\delta\left(|\vec{x}_i-\vec{x}_j| - |\vec{x}_1-\vec{x}_2|\right) \tag{1.53}$$

where i and j span the whole lattice and n is the number of different pairs of points separated by distance $|\vec{x}_2-\vec{x}_1|$. The factor 2 is because we would count any pair twice in the summation. Note that enough separation must be maintained between any pair for a given distance in order to have uncorrelated/independent pairs. Similarly for a three point correlation function $G_3(\vec{x}_1,\vec{x}_2,\vec{x}_3)$ note that the three points constitute a triangle, call it $T\{x_1,x_2,x_3\}$, and so we have

$$\begin{aligned} G_3(\vec{x}_1,\vec{x}_2,\vec{x}_3) &= \langle \varphi(\vec{x}_1)\varphi(\vec{x}_2)\varphi(\vec{x}_3)\rangle \\ &= \frac{1}{3!n'}\sum_i\sum_j\sum_k \varphi(\vec{x}_i)\varphi(\vec{x}_j)\varphi(\vec{x}_k)\delta\left(T\{x_i,x_j,x_k\} - T\{x_1,x_2,x_3\}\right) \end{aligned} \tag{1.54}$$

where the argument of the delta function is to be understood as all those points which form the triangle T, n' is the number of such triplets, and the factor 3! is to account for the over counting as before. Also as before, enough separation between triplets must be maintained to insure independence. And so on. Note how since the distribution functional has spatial and translational symmetry, only one field configuration suffices as the two point correlator is only a function of the relative distance between two points, three point correlator is only a function of the triangle formed by the triple points, and so on. However one can still, off-course, build different field realizations to obtain correlators. From here on onwards, I would refer to these random functions as fields. The structure of this report is as follows.

In the next chapter, I discuss some techniques currently in fashion to simulate these fields (usually local, homogeneous and isotropic). In chapter 3, I discuss the case of Gaussian fields and how if diagonalization transformation is known, one can trivially simulate the diagonalized field and transform it back to get the physical field. In chapter 4, I present the case of non-Gaussian fields where I show how the path integral (ground state to ground state transition) can be recast in a Markov chain that dictates generation of fields slice by slice (spatial), i.e. $N_s \to N_s$ Markov processes where N_s is the number of spatial lattice sites. For $0+1$ fields (Quantum Mechanics), Markov processes are just $1 \to 1$ (i.e. a square matrix) and I present simulations for harmonic and an-harmonic oscillator. Finally, in order to reduce the size of Markov chain in higher dimensional cases, in chapter 5 I discuss a technique that I have explored so far along with some of its simulation results.

2 Current Techniques

Consider a discrete random variable X with a set of possible outcomes $\mathcal{S}$ such that P(x) is the probability of the xth outcome in $\mathcal{S}$. Then, the basic idea is to generate a sufficiently big measure space $\mathcal{M}$ which is a collection of m independent points (or possible outcomes) such that the ratio of the number of any point x, say n_x, to the total number of points m, approaches $P(x)$. i.e.

$$\lim_{m\to\infty} \frac{n_x}{m} = P(x) \tag{2.1}$$

Then to calculate average of a quantity, say $Q(x)$, one simply calculates

$$\langle Q_x \rangle = \frac{1}{m}\sum_{i}^{m} Q(i) \tag{2.2}$$

Modelling $\mathcal{M}$ is easy for sufficiently simple probability distributions, but becomes extremely involved for many interesting distributions, specially for multi-variable distributions that I'm interested in (like functional distributions discretized to multi-variable distributions). A very commonly used technique in order to generate $\mathcal{M}$, known as Markov chain technique is discussed next.

2.1 Markov chains

Again, let X be a random variable (or a set of random variables) with probability distribution P. The basic idea is to have a Markov chain to generate the next outcome X given Y by devising a conditional probability distribution $G(X|Y)$ such that the generated outcome

is more probable to be in the high density region of P. Note that in order to ensure this, the function(al) form of G might need to be modified accordingly at regular intervals. Call them $G_1, G_2, ...$etc. Then, the sequence $\mathcal{G} = \{G_1, G_2, ..\}$ must be such, that we achieve the following property:

$$\lim_{n\to\infty} \sum_Y G_n(X|Y)P(Y) = P(X) \tag{2.3}$$

That is, the probability distribution to be achieved is the largest eigenfunction(al) of G_∞.[1] This is to ensure that at each step, outcomes obey the correct distribution P. However note that one has to then throw away many generated points/outcomes in order to un-correlate them, depending on the correlation scale of G. Then, since the measure set $\mathcal{M}$ has the right structure, ensemble average of any quantity given by

$$\langle Q \rangle = \sum_X P(X)Q(X) \tag{2.4}$$

is correctly approximated by (2.2). The convergence of G_i's to G_∞ with the property (2.3) ensures this ergodicity.

In order to ensure (2.3) for a conditional probability, one can define the following sufficient condition:

$$G(Y|X)P(X) = G(X|Y)P(Y) \tag{2.5}$$

called the condition of detailed balance, which when summed over Y, gives (2.3). Now in the case of (discretized) field theories given by an action and consequently probability distribution of the form

$$P(\vec{\varphi}) \propto e^{-S(\vec{\varphi})}, \tag{2.6}$$

[1] Although this is a sufficient condition, one can simply demand that the Markov chain $\mathcal{G}$ is irreducible, aperiodic and positive[21–24]. Then the condition (2.3) holds automatically.

the condition of detailed balance reads

$$G(\vec{\varphi}|\vec{\varphi}')e^{-S(\vec{\varphi}')} = G(\vec{\varphi}'|\vec{\varphi})e^{-S(\vec{\varphi})}. \tag{2.7}$$

Therefore it is this condition that must be satisfied by any algorithm that one wishes to devise to simulate field theories. Although there are a bunch of algorithms that are in fashion[21–25], I will describe in breif detail a very well known algorithm called as Metropolis-Hastings algorithm.

2.1.1 Metropolis- Hastings algorithm

Consider a real scalar field φ in D dimensions with a probability functional $P[\varphi]$, hence in a discrete limit given by (2.6). One starts with an arbitrary field realization $\{\vec{\varphi}\}$ and generates a new field realization $\{\vec{\varphi}'\}$ via an appropriately chosen *symmetric* conditional probability $G_o(\vec{\varphi}'|\vec{\varphi})$. Then if

$$r \equiv \frac{e^{-S(\vec{\varphi}')}}{e^{-S(\vec{\varphi})}}, \tag{2.8}$$

is ≥ 1, one keeps the new field realization. If on the other hand $r < 1$, then one keeps the new realization with a probability given by r. This can be done simply by generating a random number between 0 and 1 and keeping the new realization if this random number is smaller or equal to r. This procedure is iterated over and over to build a candidate for the sample space (to build the true sample space, one must throw away many realizations since they come out correlated, as mentioned before). Now in order to see that this procedure obeys the condition of detailed balance, note that for $r > 1$ we have for the conditional

probability G :

$$G(\vec{\varphi}'|\vec{\varphi}) = G_o(\vec{\varphi}'|\vec{\varphi}), \text{and} \tag{2.9}$$

$$G(\vec{\varphi}|\vec{\varphi}') = G_o(\vec{\varphi}|\vec{\varphi}')\frac{e^{-S(\vec{\varphi})}}{e^{-S(\vec{\varphi}')}} \tag{2.10}$$

since the probability of keeping the new point given a previous one, is the product of the probabilities of suggesting it and accepting it. The second equation above is true for the transition $\{\vec{\varphi}'\} \to \{\vec{\varphi}\}$. The two expressions give (2.7) since G_o is symmetric. Similarly for $r < 1$, we have

$$G(\vec{\varphi}'|\vec{\varphi}) = G_o(\vec{\varphi}'|\vec{\varphi})\frac{e^{-S(\vec{\varphi}')}}{e^{-S(\vec{\varphi})}}, \text{and} \tag{2.11}$$

$$G(\vec{\varphi}|\vec{\varphi}') = G_o(\vec{\varphi}|\vec{\varphi}') \tag{2.12}$$

which again gives (2.7) since G_o is symmetric. Therefore with this method, one successfully builds up the measure set $\mathcal{M}$ and to obtain average of a quantity Q, one simply calculates

$$\langle Q \rangle = \frac{1}{M}\sum_{i}^{M} Q_i \tag{2.13}$$

where i spans the measure set. The conditional probability function G_o is chosen and updated during the simulation such that the convergence to the most probable region of the distribution function P is fast enough.[2]

Due to it's dependence on the problem being tackled, estimation of the exact complexity of Metropolis algorithm is not possible in general. However, the following estimation is still possible. Let upon discretization of space and time, there be $N_s^D N$ lattice sites/random

[2]Usually for field theories, G_o is taken to be a Gaussian conditional distribution centered at the previous point.

variables where D is the number of space dimensions with N_s being the number of lattice sites in each direction, and N is the number of time lattice sites. Usually N_s is equal to N in Metropolis algorithm. Also, let after discretization of field space, the number of field values be n. Then clearly to model G_o, we need a $(n^2)^{N^{D+1}}$ matrix which is a huge matrix as N becomes larger for any given D. In each iteration then, we need to perform calculations, the number of which is of the order of $(n^2)^{N^D}$. Therefore the full complexity of any algorithm would typically be of the order of $I(n^2)^{N^{D+1}}$ where I is the number of iterations. One is typically interested in 4 dimensional field theories (3 space and 1 time direction) and therefore the complexity is $\sim I(n^2)^{N^4}$. Also, since field realizations come out correlated, one needs to throw away many field realizations which increases the number of attempts/iterations I to create the measure set and therefore the complexity even further.

In this thesis report, I present a technique which reduces the dimensionality of the problem by 1 ($D+1 \to D$), requires only one field configuration to be simulated which can be used to do statistics (due to the fact that the Lagrangian is homogeneous and isotropic). This is done by simulating a typical field configuration (D+1 dimensional) by D dimensional (spatial) slices through a Markov process obtained by massaging the path integral; instead of simulating the full $D+1$ dimensional field configurations and throwing away many of them. The complexity of the algorithm reduces to $N(n^2)^{N_s^D}$. Also, the convergence of any statistical quantity (correlators) obey central limit theorem (width $\sim 1/\sqrt{N}$). For a one dimensional problem, I present the algorithm fully where a typical field configuration is generated point by point (0 dimensional slices) via the correct conditional probability (Markov process, with complexity $\sim Nn^2$). Furthermore, the problem trivially reduces completely for Gaussian fields: any $D+1$ dimensional Gaussian field can be modeled by 0 dimensional slices (points) (complexity $\sim N_s^D N n^2$) in the similarity transformed space[3]. I

[3] this is usually the Fourier transformation

discuss the case of Gaussian fields in $D+1$ dimensions first and then finally proceed onto the more general case and reduction algorithm that we've worked on.

3 Gaussian Fields

In this chapter, I'll discuss random Gaussian fields and how we can simulate them. Two things in effect before we proceed. First, I adopt regular Particle physics unit convention (from now on throughout this thesis) where the Planck's constant $\hbar$ is set to unity; and second, since upon Wick rotation (discussed in the introduction chapter) we transition from a $D+1$ Minkowski space to a $D+1$ Euclidean space, I'll refer to the dimensionality of the space-time as D instead of $D+1$ in this section. Now consider a scalar field φ (in a D dimensional space of volume $\mathcal{V}$) with action given by

$$S = \frac{1}{2}\int\int d^D x\, d^D y\, \varphi^{\dagger}(\vec{x})\, \Delta^{-1}(\vec{x},\vec{y})\, \varphi(\vec{y}) \tag{3.1}$$

where Δ^{-1} is a symmetric function with positive spectrum (i.e. positive eigenvalues) and is invertible. This is known as a Gaussian field since there are only two non zero cumulants: mean which is zero in this case, and the two point function $\Delta(\vec{x},\vec{y})$. Now, there exists a similarity (unitary in general) transformation T (which is Fourier transformation for all our purposes) such that in the transformed representation, Δ^{-1} goes over to a diagonal matrix

$\mathcal{D}$:[1]

$$\begin{aligned}
\mathcal{D}^{-1}_{\vec{k},\vec{k}'} &= \int d^D x \int d^D y \; T_{\vec{k}}(\vec{x})\; \Delta^{-1}(\vec{x},\vec{y})\; T^{\dagger}_{\vec{k}'}(\vec{y}) = \lambda_{\vec{k}}\delta_{k,k'}, \quad \text{along with} \\
\chi_{\vec{k}} &= \int d^D x \;\; T_{\vec{k}}(\vec{x})\; \varphi(\vec{x}), \quad \text{and} \\
\delta(\vec{x}-\vec{y}) &= \sum_{\vec{k}} T^{\dagger}_{\vec{k}}(\vec{x})\, T_{\vec{k}}(\vec{y}).
\end{aligned} \tag{3.2}$$

Then, the action in the transformed representation is

$$S = \frac{1}{2}\sum_{\vec{k},\vec{k}'} \chi^{\dagger}_{\vec{k}} \mathcal{D}^{-1}_{\vec{k},\vec{k}'} \chi_{\vec{k}'} = \frac{1}{2}\sum_{\vec{k}} \chi^{\dagger}_{\vec{k}} \lambda_{\vec{k}} \chi_{\vec{k}} \tag{3.3}$$

with the following probability function for χ

$$P(\vec{\chi}) = e^{-S(\vec{\chi})}. \tag{3.4}$$

Here the vector notation is to be understood as before. Off-course in the limit $\mathcal{V} \to \infty$, k-space becomes continuous. From the probability distribution, it is evident that at each lattice point in k-space labeled by $\vec{k}$, there exists a normal random ε_t variable (complex in general) $\chi_{\vec{k}}$ with variance $1/\lambda_{\vec{k}}$:

$$\chi_{\vec{k}} = \mathcal{N}(0, 1/\lambda_{\vec{k}}). \tag{3.5}$$

One can therefore simulate the χ field pretty easily and then reverse transform it to get the physical space field φ:

$$\varphi(\vec{x}) = \sum_{\vec{k}} T^{\dagger}_{\vec{k}}(\vec{x}) \chi_{\vec{k}} \tag{3.6}$$

[1] since there is no differentiating in time and space in this section, I write only subscripts to denote discretization.

with the two point correlator equal to $\Delta = T^\dagger \mathcal{D} T$. To quickly estimate complexity of this algorithm, let, upon discretization, there be N lattice sites in each direction in k space with total number of χ field values being n. Then, total number of sites are N^D and clearly the complexity to generate a typical χ field configuration is $\sim N^D n^2$.

As a particular example, consider the well known real (Euclidean) Klein-Gordan field[4–6]. That is, a real scalar field with the following action

$$\begin{aligned} S &= \frac{1}{2}\int_{\mathcal{V}}\int_{\mathcal{V}} d^D x\, d^D y\, \varphi(\vec{x})\left[\left(-\nabla_x + m^2\right)\delta^D(\vec{x}-\vec{y})\right]\varphi(y), && (3.7)\\ &= \frac{1}{2}\int_{\mathcal{V}} d^D x\, \varphi(\vec{x})\left[-\nabla_x + m^2\right]\varphi(\vec{x}) && (3.8)\end{aligned}$$

where

$$\nabla_x \equiv \left(\frac{\partial}{\partial x^1}\right)^2 + \left(\frac{\partial}{\partial x^2}\right)^2 + \ldots \tag{3.9}$$

and the dots represent similar terms w.r.t. other directions. Then, the Fourier transformation $T_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{\mathcal{V}}} e^{i\vec{k}.\vec{x}}$ diagonalizes the Lagrangian (here, $\vec{k}.\vec{x} \equiv \sum_{i=1}^{D} k^i x^i$), and we have

$$D^{-1}_{\vec{k},\vec{k}'} = \lambda_{\vec{k}}\delta_{\vec{k},\vec{k}'} = \frac{1}{\mathcal{V}}\int d^D y \int d^D x\, e^{i\vec{k}.\vec{x}}\left[\left(-\nabla_x + m^2\right)\delta^D(\vec{x}-\vec{y})\right] e^{-i\vec{k}'.\vec{y}} = \left(\vec{k}^2 + m^2\right)\delta_{\vec{k},\vec{k}'}. \tag{3.10}$$

where off-course $\vec{k}^2 = \sum_i^D (k^i)^2$. Note that the inverse Fourier transform $T^{-1}_{\vec{k}}(\vec{x})$ is $\frac{1}{\sqrt{\mathcal{V}}} e^{-i\vec{k}.\vec{x}}$. Also then,

$$\delta(\vec{x}-\vec{y}) = \frac{1}{\mathcal{V}}\sum_{\vec{k}} e^{i\vec{k}.(\vec{x}-\vec{y})}. \tag{3.11}$$

With this, action in Fourier space becomes

$$S = \frac{1}{2}\sum_{\vec{k}} \chi^*_{\vec{k}}\left(\vec{k}^2 + m^2\right)\chi_{\vec{k}} \tag{3.12}$$

with

$$P(\vec{\chi}) = \exp\left\{ -\frac{1}{2}\sum_{\vec{k}} \chi^*_{\vec{k}} \left(k^2 + m^2\right) \chi_{\vec{k}} \right\}, \tag{3.13}$$

i.e. in Fourier space at each lattice site, we have a random Gaussian variable $\chi_{\vec{k}} = \mathcal{N}(0, 1/(\vec{k}^2 + m^2))$. Note that since φ is real, we must have $\chi^*_{\vec{k}} = \chi_{-\vec{k}}$. We can then obtain φ by simulating χ and then Fourier transforming it:

$$\varphi(x) = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\vec{k}} e^{ik.x} \chi_{\vec{k}}. \tag{3.14}$$

Note that the two point correlator is

$$\langle \varphi(x)\varphi(y) \rangle = \left[\left(-\nabla_x + m^2\right) \delta^D(x-y) \right]^{-1} = \frac{1}{\mathcal{V}} \sum_{\vec{k}} \frac{e^{ik.(x-y)}}{k^2 + m^2} \tag{3.15}$$

which, in the large volume limit and working in angular variables ($\sum_{\vec{k}} \to \frac{\mathcal{V}}{(2\pi)^D} \int d^D k$) becomes

$$\frac{1}{(2\pi)^D} \int d^D k \, \frac{e^{ik.(x-y)}}{k^2 + m^2}. \tag{3.16}$$

To illustrate things more specifically, consider the real scalar one dimensional Klein-Gordan field $\varphi(x)$ which is nothing but a harmonic oscillator. The action

$$S = \frac{1}{2} \int dx \left[\left(\frac{d\varphi}{dx} \right)^2 + m^2 \varphi^2 \right] \tag{3.17}$$

in Fourier space has the form

$$S = \frac{1}{2} \sum_k \chi^*_k \left(k^2 + m^2\right) \chi_k \tag{3.18}$$

and therefore

$$P = \exp\left\{ -\frac{1}{2}\sum_k \left(k^2 + m^2\right) \chi_k^* \chi_k \right\} \tag{3.19}$$

Now as pointed out before, $\chi_{-k}^* = \chi_k$ since φ is real. Denoting $\chi_k = a_k + i b_k$, this means we have $a_k = a_{-k}$ and $b_k = -b_{-k}$. Therefore we need to only worry about one half of the k-spectrum since the other depends on it. Further, let the physical box (1-D line) size be L and its discretization step be ε. Then requiring periodic boundary conditions, we have $k = 2\pi n/L$ where $n \in I$ and we must impose a UV cutoff (a maximum n) by requiring that the maximum magnitude of k be of the order of $2\pi/\varepsilon$. Then let the number of positive k values be N (total then being $2N+1$). The probability distribution in k-space with all this is

$$\begin{aligned} P &= \exp\left\{ -\frac{1}{2}\sum_{n=0}^{N} \left(\left(\frac{2\pi n}{L}\right)^2 + m^2 \right) (a_k)^2 \right\} \exp\left\{ -\frac{1}{2}\sum_{n=1}^{N} \left(\left(\frac{2\pi n}{L}\right)^2 + m^2 \right) (b_k)^2 \right\} \\ &\times \prod_{n=1}^{N} \delta(a_n - a_{-n}) \prod_{n=0}^{N} \delta(b_n + b_{-n}). \end{aligned} \tag{3.20}$$

That is at each point in the positive k-space, we have two Gaussian random numbers a_k and b_k, equal to $\mathcal{N}\left(0, \frac{1}{(2\pi n/L)^2 + m^2}\right)$ with the negative half determined by $a_{-k} = a_k$ and $b_{-k} = -b_k$. The physical φ field is then obtained by inverse Fourier transformation of $\chi_k = a_k + i b_k$:

$$\varphi_x = \frac{1}{\sqrt{L}} \sum_k e^{ikx} \chi_k \tag{3.21}$$

where off-course the summation runs through all of the k values. Similarly, we can extend this discussion to higher dimensional cases. Simulating Gaussian fields is therefore quite trivial once we know what the similarity transformation is. Although things get quickly involved when we have non-Gaussian fields since there does not exist any linear transformation that diagonalizes the Lagrangian, there exists at least one way to re-write the path

integral/probability distribution that can potentially reduce the complexity of the problem. This I discuss in the next chapter.

4 Non-Gaussian fields

Consider a $D+1$ dimensional real scalar field with the following action

$$S = \int dt\, d^D x \left((\partial\varphi)^2 + \frac{1}{2} m^2 \varphi^2 + \lambda V(\varphi) \right) \tag{4.1}$$

where $(\partial\varphi)^2$ is a shorthand notation for $(\partial\varphi/\partial t)^2 + (\partial\varphi/\partial x^1)^2 + ...$, and V is some non-quadratic concave up function of φ, in the discretized version. Then, given a state $\Psi_t(\vec{\varphi}')$ at time t, at the next time step we have

$$\Psi_{t+\varepsilon}(\vec{\varphi}) = \int D[\vec{\varphi}'] K_E(\vec{\varphi}, t+\varepsilon; \vec{\varphi}', t) \Psi_t(\vec{\varphi}') \tag{4.2}$$

where K_E is (c.f. (1.40) and (1.41))

$$K_E(\vec{\varphi}, t+\varepsilon, \vec{\varphi}', t) = \left(\sqrt{\frac{1}{2\pi\varepsilon^D}} \right)^N e^{-S_d} \tag{4.3}$$

and d stands for discretized. This means that for any nth eigenstate of the kernel, we have

$$\Psi_n(\vec{\varphi}) = e^{-\varepsilon E_n} \int D[\vec{\varphi}'] K_E(\vec{\varphi}, t+\varepsilon; \vec{\varphi}', t) \Psi_n(\vec{\varphi}'). \tag{4.4}$$

Building up on this (and absorbing $e^{-\varepsilon E_0}$ in redefining $\tilde{K}_E$ as before), ground to ground state transition from t_0 to t_N is

$$\begin{aligned}\langle 0|\tilde{U}(t_N,t_0)|0\rangle &= \prod_{i=0}^{N}\int D[\vec{\varphi}_i]\psi_0(\vec{\varphi}_N)\,\tilde{K}_E\left(\vec{\varphi}_N,t_N;\vec{\varphi}_{N-1},t_{N-1}\right)...\tilde{K}_E\left(\vec{\varphi}_1,t_1;\vec{\varphi}_0,t_0\right)\psi_0(\vec{\varphi}_0)\\ &= \prod_{i=0}^{N}\int D[\vec{\varphi}_i]\psi_0(\vec{\varphi}_N)\,\tilde{K}_E\left(\vec{\varphi}_N,\vec{\varphi}_{N-1},\varepsilon\right)...\tilde{K}_E\left(\vec{\varphi}_1,\vec{\varphi}_0,\varepsilon\right)\psi_0(\vec{\varphi}_0)\\ &= \prod_{i=0}^{N}\int D[\vec{\varphi}_i]\;P(\vec{\varphi}_N,\vec{\varphi}_{N-1},...,\vec{\varphi}_0)=1 \qquad (4.5)\end{aligned}$$

where in the second line I have replaced time steps $t_k - t_{k-1}$ by ε since kernel only depends on the time difference. Now, this probability distribution can be recast by multiplying and dividing by the ground state wave-function(al) at each successive time steps[1]:

$$\begin{aligned}P(\vec{\varphi}_N,\vec{\varphi}_{N-1},...,\vec{\varphi}_0) = &\left(\frac{\psi_0(\vec{\varphi}_N)\,\tilde{K}_E\left(\vec{\varphi}_N,\vec{\varphi}_{N-1},\varepsilon\right)}{\psi_0(\vec{\varphi}_{N-1})}\right)\left(\frac{\psi_0(\vec{\varphi}_{N-1})\,\tilde{K}_E\left(\vec{\varphi}_{N-1},\vec{\varphi}_{N-2},\varepsilon\right)}{\psi_0(\vec{\varphi}_{N-2})}\right)...\\ &\left(\frac{\psi_0(\vec{\varphi}_2)\,\tilde{K}_E\left(\vec{\varphi}_2,\vec{\varphi}_1,\varepsilon\right)}{\psi_0(\vec{\varphi}_1)}\right)\left(\frac{\psi_0(\vec{\varphi}_1)\,\tilde{K}_E\left(\vec{\varphi}_1,\vec{\varphi}_0,\varepsilon\right)}{\psi_0(\vec{\varphi}_0)}\right)\psi_0^2(\vec{\varphi}_0) \qquad (4.6)\end{aligned}$$

Here, the objects in brackets integrate to 1 when integrated over the first variable(s) since $\Psi_0(\vec{\varphi}_k)$ is an eigenfunction of $K_E\left(\vec{\varphi}_k,\vec{\varphi}_{k-1},\varepsilon\right)$ with eigenvalue 1[2]; and are also positive definite since both the ground state wave-function(al) Ψ_0 and K_E are positive definite. Therefore:

$$\mathcal{P}_\varepsilon\left(\vec{\varphi}_k|\vec{\varphi}_{k-1}\right) \equiv \frac{\psi_0(\vec{\varphi}_k)\,\tilde{K}_E\left(\vec{\varphi}_k,\vec{\varphi}_{k-1},\varepsilon\right)}{\psi_0(\vec{\varphi}_{k-1})} \qquad (4.7)$$

is a valid conditional probability distribution function(al). Now since K_E is symmetric, the conditional probability distribution has the density function $\rho\left(=\Psi_0^2\right)$ as its eigenfunction

[1] This idea of multiplication and division by dominant eigenstate was proposed by Dr. Vitaly Vanchurin in an unpublished work on multi-variable probability distributions and conditional probabilities.

[2] This is true since K_E is symmetric.

with eigenvalue 1:

$$\begin{aligned}\int D[\vec{\varphi}_{k-1}]\mathcal{P}_\varepsilon(\vec{\varphi}_k|\vec{\varphi}_{k-1})\,\psi_0^2(\vec{\varphi}_{k-1}) &= \psi_0(\vec{\varphi}_k)\int D[\vec{\varphi}_{k-1}]\tilde{K}_E(\vec{\varphi}_k,\vec{\varphi}_{k-1},\varepsilon)\,\psi_0(\vec{\varphi}_{k-1}) \\ &= \psi_0^2(\vec{\varphi}_k) \qquad (4.8)\end{aligned}$$

Finally with this, the probability distribution P is a sequence of conditional probabilities $\mathcal{P}$ with ρ in the beginning (which won't matter in the large bulk limit as pointed out in chapter 1):

$$P(\vec{\varphi}_N,\vec{\varphi}_{N-1},...,\vec{\varphi}_0) = \mathcal{P}_\varepsilon(\vec{\varphi}_N|\vec{\varphi}_{N-1})...\mathcal{P}_\varepsilon(\vec{\varphi}_1|\vec{\varphi}_0)\,\psi_0^2(\vec{\varphi}_0) \qquad (4.9)$$

and therefore the ground to ground transition is a Markov chain:

$$\langle 0|\tilde{U}(t_N,t_0)|0\rangle = \prod_{i=0}^{N}\int D[\vec{\varphi}_i]\mathcal{P}_\varepsilon(\vec{\varphi}_N|\vec{\varphi}_{N-1})...\mathcal{P}_\varepsilon(\vec{\varphi}_1|\vec{\varphi}_0)\,\psi_0^2(\vec{\varphi}_0) = 1 \qquad (4.10)$$

What is dictated by this Markov chain is that at each step/time slice, the random variable(s) are drawn from the density function ρ and are correlated by the conditional probability $\mathcal{P}$ which is exactly what we should have if we wish to generate typical field configurations ($D+1$ dimensional) from ground state to ground state through D dimensional slices. For the estimation of complexity of the algorithm, let the number of time steps be N and the number of spatial lattice sites in each direction be N_s. Also let the number of field values upon discretization of field space be n. Then clearly, $\mathcal{P}$ is a $(n^2)^{N_s^D}$ matrix and the total number of computations (complexity) are $\sim N(n^2)^{N_s^D}$. Also since we pick $\{\vec{\varphi}\}$'s from the correct distribution (ρ) with proper correlations (as dictated by the ground to ground Markov chain i.e. a sequence of $\mathcal{P}_\varepsilon$'s), the convergence of any statistical quantity (for example the two point correlator) to the actual one simply goes in accordance with the central limit theorem (width $\sim 1/\sqrt{N}$).

In the next section, I discuss the case of $0+1$ scalar field (quantum mechanics) with some simulation results for harmonic and an-harmonic oscillator.[3]

4.1 $D = 0$ (Non-relativistic Quantum Mechanics)

In 0 space dimensions, things get fairly simplified. Consider a system with Euclidean action $S[\varphi]$ given as

$$S = \int dt \left(\left(\frac{d\varphi}{dt} \right)^2 + \frac{1}{2} m^2 \varphi^2 + \lambda V(\varphi) \right) \tag{4.11}$$

Then, as per the above discussion, the conditional probability is

$$P_\varepsilon(\varphi_k | \varphi_{k-1}) = \frac{\psi_0(\varphi_k)\, \tilde{K}_E(\varphi_k, \varphi_{k-1}, \varepsilon)}{\psi_0(\varphi_{k-1})} \tag{4.12}$$

where off course ψ_0 is the ground state wave function and K_E is the kernel with distribution function ρ $(= \psi_0^2)$ as its eigenvector. With this we can create a typical field configuration point by point through this conditional probability. As a first example, consider harmonic oscillator ($\lambda = 0$) with

$$S = \int dt \left(\left(\frac{d\varphi}{dt} \right)^2 + \frac{1}{2} m^2 \varphi^2 \right) \tag{4.13}$$

in the discretized version. That is, the kernel is

$$\tilde{K}_E(\varphi_k, \varphi_{k-1}, \varepsilon) = \frac{1}{\sqrt{2\pi\varepsilon}} \exp\left[-\frac{\varepsilon}{2} \left(\left(\frac{\varphi_k - \varphi_{k-1}}{\varepsilon} \right)^2 + m^2 \left(\frac{\varphi_k + \varphi_{k-1}}{2} \right)^2 \right) \right] \tag{4.14}$$

[3] The case of $0+1$ fields was already under ongoing investigations by Hadi Papei, in collaboration with Vitaly Vanchurin and Yi-Zen Chu

where (as before) I have thrown the potential in between the two lattice sites to keep the discretized kernel symmetric (c.f. (1.21)). The ground state is well known and is equal to

$$\psi_0(\varphi) = \left(\frac{m^2}{2\pi}\right)^{1/4} \exp\left(-\frac{m}{2}\varphi^2\right). \tag{4.15}$$

In this case therefore, we have an analytic expression for the conditional probability function:

$$\mathcal{P}_\varepsilon(\varphi_k|\varphi_{k-1}) = \frac{\psi_0(\varphi_k)\,\tilde{K}_E(\varphi_k,\varphi_{k-1},\varepsilon)}{\psi_0(\varphi_{k-1})} = \frac{\exp\left(\frac{m\varepsilon}{2}\right)}{\sqrt{2\pi\varepsilon}} \exp\left[\frac{\varepsilon}{2}\left(\frac{\varphi_k-\varphi_{k-1}}{\varepsilon} + m\frac{\varphi_k+\varphi_{k-1}}{2}\right)^2\right] \tag{4.16}$$

Note that this corresponds to a Gaussian process for which the Langevin equation (in the discrete version) is

$$\frac{\varphi_j-\varphi_{j-1}}{\varepsilon} + m\frac{\varphi_j+\varphi_{j-1}}{2} = \eta_{j-1} \tag{4.17}$$

where η is a random Gaussian variable $\mathcal{N}(0,\sqrt{\varepsilon})$. Creating a typical field then, simply requires us to start with a random field value φ_0, and then picking the next as dictated by (4.16) or equivalently by (4.17), at each subsequent step. In general, finding the ground state of a Kernel (which is basically just an $n \times n$ matrix for simulation purposes where n is the number of points/values in field space) is a really simple task. Since the ground state is also the dominant eigenvector of the Kernel, one can start with any arbitrary state in the beginning and apply kernel successively to it until the desired accuracy is attained. Now as pointed out earlier in Chapter 1, one can calculate all possible moments (correlation functions) from this typical field configuration since the field is isotropic and homogeneous. As an example, two point correlator $\langle\varphi(t_2)\varphi(t_1)\rangle$ can be calculated by taking all pairs of points (sufficiently far apart so that they are uncorrelated) with separation $|t_2-t_1|$ and averaging over their products. To compare numerics with analytics, note that theoretically,

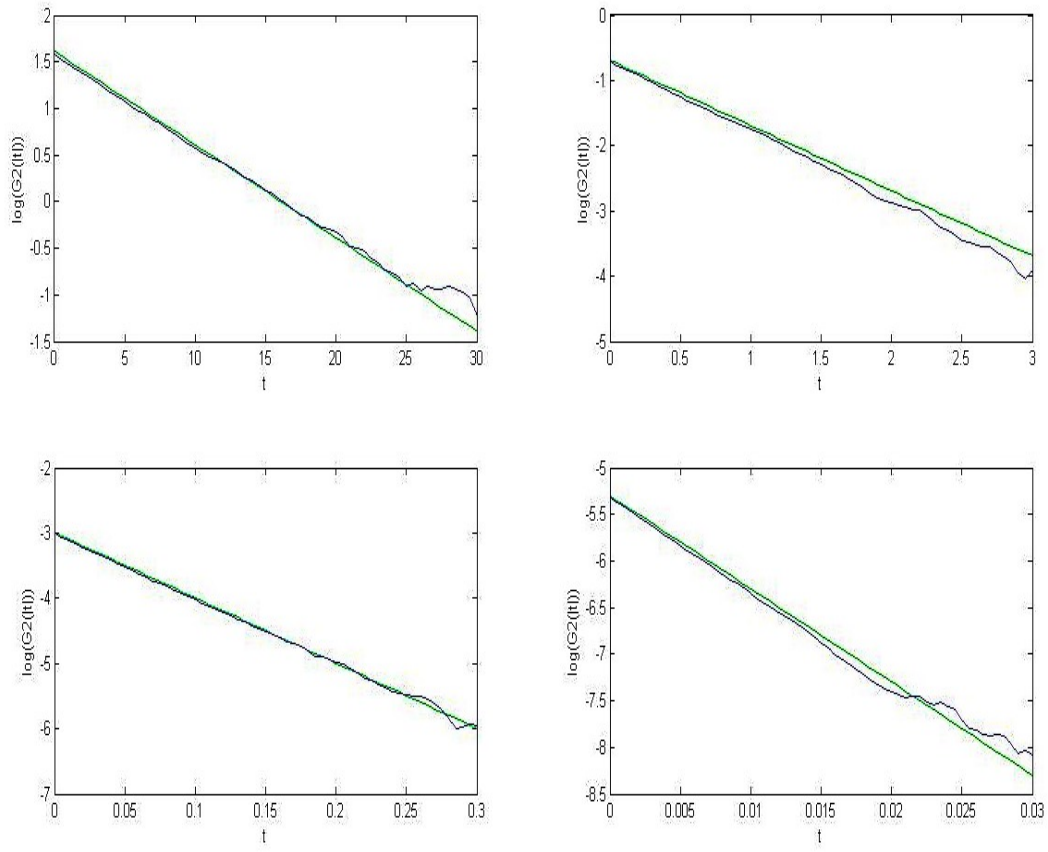

Figure 4.1: Here, the green and blue plots are analytical and numerical for masses 0.1, 1, 10 and 100 respectively. Y axis is natural log of (4.18) ($\ln\langle\varphi(t_2)\varphi(t_1)\rangle_{theory}$) and x axis is the distance ($|t_2-t_1|$) with the extent of x axis being $3/\text{mass}$.

the two point correlator in the continuous time limit (3.16) is easily evaluated to be

$$\langle\varphi(t_2)\varphi(t_1)\rangle_{theory} = \frac{1}{2\pi}\int dk\,\frac{e^{ik(t_2-t_1)}}{k^2+m^2} = \frac{1}{2m}e^{-m|t_2-t_1|}. \tag{4.18}$$

through complex-contour integration. Figure 4.1 compares the numerical and analytical natural log of correlation function for masses $m = 0.1, 1, 10, 100$[4]. Moving on, now con-

[4]Hadi Papei's subsequent final simulations (unpublished), were later found to be in agreement with these results. See[26] for Hadi's initial 2016 APS conference presentation

sider a an-harmonic oscillator ($\lambda \neq 0$):

$$S = \int dt \left(\left(\frac{d\varphi}{dt} \right)^2 + \frac{1}{2} m^2 \varphi^2 + \lambda \varphi^4 \right) \tag{4.19}$$

for which K_E in the discretized limit is

$$\tilde{K}_E(\varphi_k, \varphi_{k-1}, \varepsilon) = \frac{1}{\sqrt{2\pi\varepsilon}} \exp\left[-\frac{\varepsilon}{2} \left(\left(\frac{\varphi_k - \varphi_{k-1}}{\varepsilon} \right)^2 + m^2 \left(\frac{\varphi_k + \varphi_{k-1}}{2} \right)^2 + 2\lambda \left(\frac{\varphi_k + \varphi_{k-1}}{2} \right)^4 \right) \right] \tag{4.20}$$

Note that because of the non-linearity of the system, a full analytical calculation of any eigenvector of this kernel is impossible. However for $\lambda << m^3$, one usually employs perturbation techniques and calculates all the desired quantities (eigenvectors, ground to ground correlators, etc.) in a power series in the perturbing parameter λ. This is a very well known and standard technique[4–6] that I won't dwell on. As a particular case, the two point correlator up to first order in λ (i.e. terms involving λ^0 and λ^1 only) is given by

$$\langle x(t_2) x(t_1) \rangle_{theory} = \frac{1}{2m} e^{-m|t_2 - t_1|} \left[1 - \frac{3\lambda}{m^2} \left(|t_2 - t_1| + \frac{1}{m} \right) + O(\lambda^2) \right] \tag{4.21}$$

For numerics, we obtain ψ_0 as explained above up to the desired accuracy and then define (4.12) to generate a field configuration point by point. Figure 4.2 below compares the analytical (up to first order terms in λ) and numerical two point correlators for $\lambda = 0.05 * \text{mass}^3$ for the above four masses. With this understanding, we can now easily go beyond the perturbative regime (that is $\lambda > 1$) where analytical calculation is forbidden and obtain all correlators. The complexity, since $D = 0$, is simply $N(n \times n)$ where N is the number of lattice sites in the time direction (time steps).

All this can be easily extended to larger systems. For example, consider the following

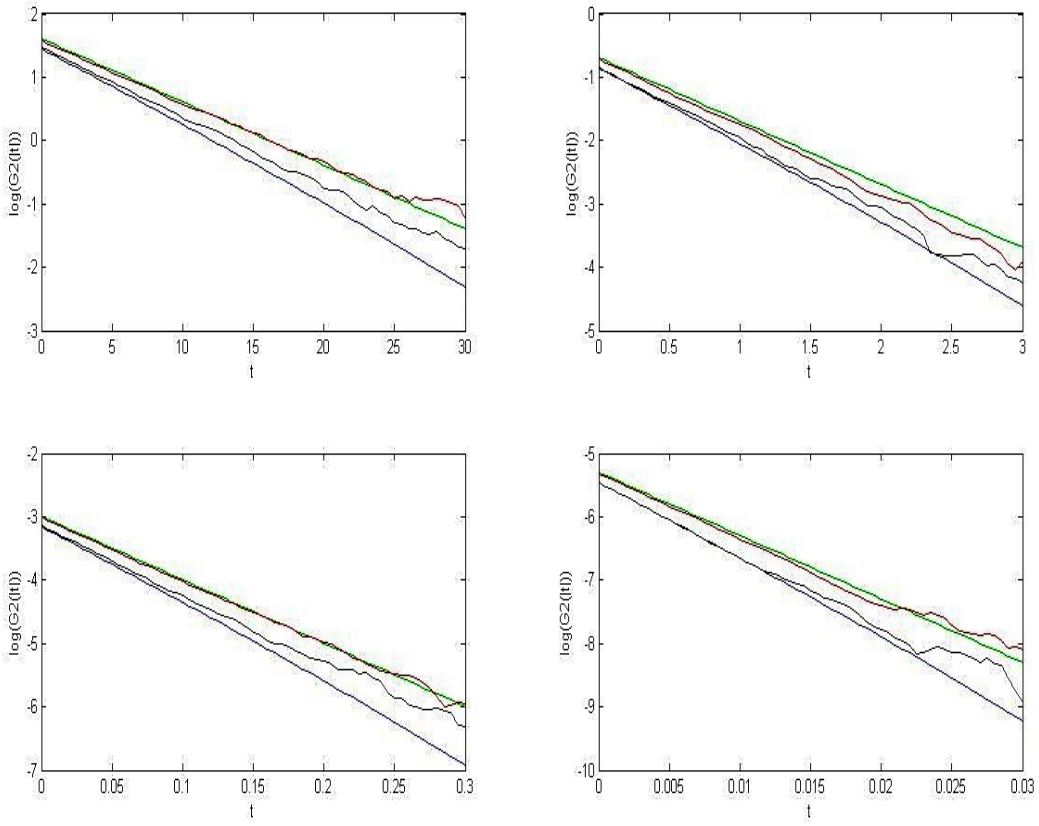

Figure 4.2: Here as before, green and blue plots are for free theory (analytical and numerical respectively) while blue and black are for interacting theory (analytical and numerical respectively).

action

$$S = \int dt \left(\frac{1}{2} \left(\frac{d\varphi}{dt} \right)^2 + \frac{1}{2} \left(\frac{d\xi}{dt} \right)^2 + V(\varphi, \xi) \right) \tag{4.22}$$

where φ and ξ denote two $(0+1)$ fields or positions of two particles, and V is any potential function of the two fields. The discretized Euclidean kernel and conditional probability

function are respectively

$$\tilde{K}_E(\varphi_k,\xi_k,\varphi_{k-1},\xi_{k-1},\varepsilon) = \frac{1}{2\pi\varepsilon}\exp\left[-\varepsilon\left(\frac{1}{2}\left(\frac{\varphi_k-\varphi_{k-1}}{\varepsilon}\right)^2+\frac{1}{2}\left(\frac{\xi_k-\xi_{k-1}}{\varepsilon}\right)^2+V\left(\frac{\varphi_k+\varphi_{k-1}}{2},\frac{\xi_k+\xi_{k-1}}{2}\right)\right)\right] \tag{4.23}$$

and

$$\mathcal{P}_\varepsilon(\varphi_k,\xi_k\,|\,\varphi_{k-1},\xi_{k-1}) = \frac{\psi_0(\varphi_k,\xi_k)\,\tilde{K}_E(\varphi_k,\xi_k,\varphi_{k-1},\xi_{k-1},\varepsilon)}{\psi_0(\varphi_{k-1},\xi_{k-1})} \tag{4.24}$$

with ψ_0 being the ground state wave-function. As it is evident, this is a 2 to 2 ($\{\varphi,\xi\}\rightarrow\{\varphi,\xi\}$) Markov process. If the potential function is such that it doesn't contain any mixed terms of φ and ξ, then we have a decoupled system and clearly, the $2\rightarrow 2$ Markov process reduces to two $1\rightarrow 1$ Markov processes. On extending the discussion further by adding more and more degrees of freedom (more such fields), say N_s of them, one gets to the case of 1 or more (spatial-) dimensional field theories, and the conditional probability function becomes a huge function (equivalently the Markov process becomes huge: $N_s\rightarrow N_s$). However if all these (0+1) fields decouple, then $\mathcal{P}$ is just a product of individual $\mathcal{P}$'s for each $(0+1)$ field (equivalently Markov process reduces to N_s one to one processes) and everything becomes trivial and easy to manage. This is exactly the case of a Gaussian ($D\geq 1$) field that I discussed in the previous chapter with the difference being that here I would Fourier decompose only the spatial lattice and therefore each point in k-lattice becomes a one to one Markov process. Whereas on the other hand if there are couplings within some subset, there remains a portion of the full Markov process which does not reduce completely (i.e. $\mathcal{P}$ does not completely reduce to product of individual $\mathcal{P}$'s) and handling it then requires heavy computational machinery (parallel processing).

4.2 $D \geq 1$

As a simple example, consider a $1+1$ Gaussian (real Klein-Gordon) field in physical space with the familiar action

$$S = \int dt\, dx \left[\frac{1}{2} \left(\frac{\partial \varphi}{\partial t} \right)^2 - \frac{1}{2} \left(\frac{\partial \varphi}{\partial y} \right)^2 - \frac{1}{2} m^2 \varphi^2 \right]. \tag{4.25}$$

The ground state wave functional is easily written in the k-space as

$$\Psi[\varphi] \propto \exp\left\{ -\frac{1}{2V} \sum_k \sqrt{k^2 + m^2}\, |\varphi_k|^2 \right\} \tag{4.26}$$

since all we have is a bunch of harmonic oscillators (4.15). This however, in the physical space has the form

$$\exp\left\{ -\frac{1}{2} \int dx\, dy\, \varphi(x)\, D(|x-y|)\, \varphi(y) \right\} \tag{4.27}$$

where D, defined to be

$$D(|x-y|) \equiv \frac{1}{V} \sum_k e^{ik(x-y)} \sqrt{k^2 + m^2} \tag{4.28}$$

has support over all lattice sites (on discretized space off-course) and not just nearby ones, dictating a non-locality. Hence we have a $N_s \to N_s$ Markov process, say $\mathcal{P}_\varepsilon(\vec{\varphi}_N | \vec{\varphi}_{N-1})$, where N_s is off-course the number of spatial lattice sites upon discretization. This can be pictorially represented as what is known as a *Bayesian* network, shown in figure 1. Note that the non-locality and the fact that the full Markov process does not reduce to any simpler one (in physical space), is due to the presence of the *spatial derivative* coupling in the Lagrangian. If that were not present, we would have decoupled $(1-1)$ Markov processes at each lattice site (as is true in k-space for Gaussian fields). Now, if one has such a numerical ability to model large Markov processes, then I am basically done and we've successfully

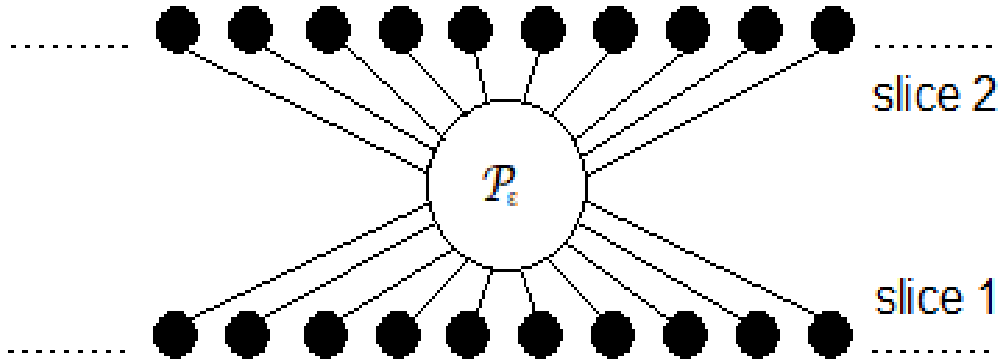

Figure 4.3: A checkerboard network. As must be self-evident, black dots represent lattice sites and solid lines represent connections.

reduced the dimensionality of the problem of simulating fields numerically, by 1. This however is not our final goal as we want to reduce the problem for non-Gaussian fields in higher dimensions (if at all possible) to an extent that heavy computational machinery is not required. If not, then we want to search for a no-go theorem proving that such a reduction is not possible. This is currently under investigation. In the next chapter, I discuss some of the potential techniques and discuss one particular Bayesian network that I have investigated so far along with some simulation results.

5 Bayesian networks: A test checkerboard network

Perhaps naively, one might think not to have too many spatial lattice points. But since the discretization step of spatial lattice depends on the correlation length (there must be enough lattice sites within correlation length with discretization small enough that correlations stay almost constant within each step), to have enough precision one usually requires a large enough/non-local (that must connect far away lattice sites and not just nearby ones) conditional probability $\mathcal{P}$ that guarantees reproduction of correlations correctly. Specifically (for a homogeneous and isotropic field), having N_s spatial lattice sites within a correlation length in each direction (with the box size in each spatial direction equal to only the correlation length) would require $\mathcal{P}$ to be a $2 \times N_s^D$ argument function which is quite huge even for $N_s = 5$ and $D = 3$ (equal to 250) due to exponential dependence on D (equivalently a 125 to 125 Markov process). If this is doable, then eventually (long time run) we will converge to the ground state ρ of $\mathcal{P}$ (equal to the square of the ground state of kernel) with others exponentially suppressed as explained before in Chapter 4. That is,

$$\int D[\vec{\varphi}_k]\, \mathcal{P}(\vec{\varphi}_{k+1}|\vec{\varphi}_k)\, \rho(\vec{\varphi}_k) = \rho(\vec{\varphi}_{k+1}) \tag{5.1}$$

Now, the main idea is to somehow construct some sufficiently local conditional probability, say P_{sub}, that only connects nearby lattice sites and then mix different lattice sites in some fashion in order to correlate them back. Now such a strategy would require us to insert

some auxiliary slices in between any two physical spatial slices in order to correlate sites that weren't before due to locality of P_{sub}'s, which would eventually be thrown away once the transition from one physical slice to next is made. More concretely, we want to massage the above equation in the following form

$$\int D[\vec{\varphi}_k]\, D[\vec{\varphi}_{aux1}] ... D[\vec{\varphi}_{auxn}]\, P^{(n)}_{sub}(\vec{\varphi}_{k+1}|\vec{\varphi}_{auxn}) ... P^{(2)}_{sub}(\vec{\varphi}_{aux2}|\vec{\varphi}_{aux1})\, P^{(1)}_{sub}(\vec{\varphi}_{aux1}|\vec{\varphi}_k)\, \rho(\vec{\varphi}_k) = \rho(\vec{\varphi}_{k+1}) \quad (5.2)$$

where the vector notation is to be understood as explained before in chapter 1. Here, different local P_{sub}'s (with superscripts) have different connections (in order to correlate far away points), since any one would only connect nearby ones.[1] Finding any set of P_{sub}'s analytically that solves the problem is challenging and seems formidable at this point. Therefore, we resort to coming up with different P_{sub}'s and testing them numerically to at least guide us better. I discuss next a 2-2 network (i.e. having local 2-2 Markov processes) that we call a checkerboard network, in detail.

5.1 Checkerboard network

Here, only one auxiliary slice is needed. The basic idea is to group every two adjacent lattice sites together, propagate them via some conditional probability P_{sub} to generate an auxiliary slice, and then in the next step to generate the second physical slice, shift the grouping by one site either to the left or right. And repeat. For example, if the groupings were $(k,k+1),(k+2,k+3),...$ where k denotes the kth lattice site, then in the next propagation the grouping will be $(k-1,k),(k+1,k+2)...$ and so on (see figure 5.1). The actual slice to slice propagation is then via the conditional probability $\mathcal{P}'$ denoted in terms

[1] Such a reduction may not even be possible depending on how much locality one desires, something that I'm currently investigating

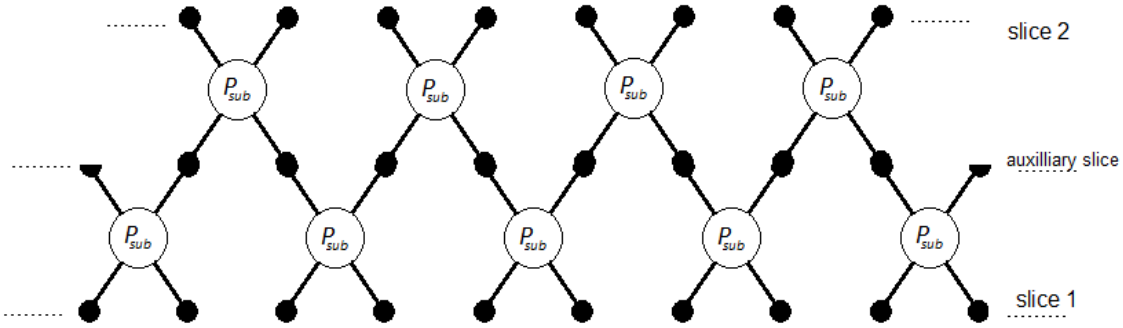

Figure 5.1: A checkerboard network. As must be self-evident, black dots represent lattice sites and solid lines represent connections.

of P_{sub} as $\{P_{sub}\}_1 \cdot \{P_{sub}\}_2$ where 1 and 2 denote the two steps (slice 1 to auxiliary to slice 2) with the two different groupings respectively. Note that the network so generated is homogeneous by construction which is a property we desire off-course. Also, due to homogeneity, two point correlators along different directions can be found from a typical field configuration so generated, by averaging over two point correlators for each 1 dimensional slice (straight lines) along the desired direction found as before for a 1-D case. By finding two point correlators along different directions, we can know whether the field generated is isotropic or not for a given P_{sub}. Although there is in principle an infinite space of 2 to 2 conditional probabilities one can try to construct, I describe one particular P_{sub} that we have worked with so far. I'll construct this next for a $1+1$ Klein Gordon field[2] and show graphs of a typical field generated and correlators in different directions in this field configuration, to see how much of the isotropy is achieved.

[2]having a non-Gaussian field is not necessary for any network. In principle, it is obvious that a network must be able to simulate any $V(\varphi)$ since the main objective is to capture the spatial derivative coupling. However for the purpose of illutration, I work with the simple case of a Klein-Gordon field

5.2 A test conditional probability and its network

Consider a 2-2 (having only two spatial sites) Klein Gordon kernel:

$$K(\varphi^i_{j+1},\varphi^{i+1}_{j+1},\varphi^i_j,\varphi^{i+1}_j)=\exp\left[-\frac{\varepsilon_t\,\varepsilon_x}{4}\left(\left(\frac{\varphi^i_{j+1}-\varphi^i_j}{\varepsilon_t}\right)^2+\left(\frac{\varphi^{i+1}_{j+1}-\varphi^{i+1}_j}{\varepsilon_t}\right)^2+\left(\frac{\varphi^{i+1}_{j+1}-\varphi^i_{j+1}}{\varepsilon_x}\right)^2+\left(\frac{\varphi^{i+1}_j-\varphi^i_j}{\varepsilon_x}\right)^2+m^2\left(\frac{\varphi^i_{j+1}+\varphi^{i+1}_{j+1}+\varphi^i_j+\varphi^{i+1}_j}{4}\right)^2\right)\right]. \quad (5.3)$$

where as usual, superscript and subscript indices label the lattice site (with discretization ε_x) at each time step, and time step (with discretization ε_t) at each lattice site respectively. The first two terms dictate time interactions at each spatial site and the second two dictate spatial interactions at each time step. The last term is the potential term which in this case is just a quadratic potential. Now for this simple 2-2 network, we can actually find the ground state analytically by breaking the 2-2 process into two decoupled 1-1 processes by switching to the center of mass $\xi_j \equiv (\varphi^i_j+\varphi^{i+1}_j)/2$ and difference coordinates $\eta_j=(\varphi^i_j-\varphi^{i+1}_j)/2$ at each time step. In these coordinates, the above kernel becomes

$$\exp\left[-\frac{\varepsilon_t\,\varepsilon_x}{2}\left(\left(\frac{\xi_{j+1}-\xi_j}{\varepsilon_t}\right)^2+\left(\frac{m}{\sqrt{2}}\right)^2\left(\frac{\xi_{j+1}+\xi_j}{2}\right)^2+\left(\frac{\eta_{j+1}-\eta_j}{\varepsilon_t}\right)^2+\left(\frac{2}{\varepsilon_x}\right)^2\left(\frac{\eta^2_{j+1}+\eta^2_j}{2}\right)\right)\right]. \quad (5.4)$$

Clearly, the difference coordinate is a harmonic oscillator and the center of mass coordinate is whatever depending upon the potential V (here also, harmonic oscillator). That is, we have two decoupled harmonic oscillators for which we can easily write the ground state

(c.f. (4.15)) and then convert back to the original coordinates:

$$\begin{aligned}\psi_0'(\varphi_j^{i+1},\varphi_j^i) &\propto \exp\left(-\frac{m\varepsilon_x}{2\sqrt{2}}\,\xi_j^2\right)\exp\left(-\eta_j^2\right)\\ &= \exp\left(-\frac{m\varepsilon_x}{2\sqrt{2}}\left(\frac{\varphi_j^{i+1}+\varphi_j^i}{2}\right)^2\right)\exp\left(-\left(\frac{\varphi_j^{i+1}-\varphi_j^i}{2}\right)^2\right). \qquad (5.5)\end{aligned}$$

The respective conditional probability is

$$p_{sub}(\varphi_{j+1}^{i+1},\varphi_{j+1}^i|\varphi_j^{i+1},\varphi_j^i)=\frac{\psi_0'(\varphi_{j+1}^{i+1},\varphi_{j+1}^i)\,K(\varphi_{j+1}^{i+1},\varphi_{j+1}^i,\varphi_j^{i+1},\varphi_j^i)}{\psi_0'(\varphi_j^{i+1},\varphi_j^i)}\equiv p_{(i+1,i)}, \qquad (5.6)$$

which is the one block (2 sites to 2 sites) conditional probability for the checkerboard network. The full $\mathcal{P}'$ for a physical slice $\vec{\varphi}_{k+1}$ to physical slice $\vec{\varphi}_k$ transition with a auxiliary slice $\vec{\varphi}_{aux}$ (that is to be thrown away) is therefore

$$\begin{aligned}\mathcal{P}' &\equiv \{P_{sub}\}_1\cdot\{P_{sub}\}_2=\int D[auxiliary\ slice]\left(\prod_i p_{(2i,2i-1)}\right)\left(\prod_i p_{(2i+1,2i)}\right)\\ &= \int D[\vec{\varphi}_{aux}]\,P_{sub}(\vec{\varphi}_{k+1}|\vec{\varphi}_{aux})\,P_{sub}(\vec{\varphi}_{aux}|\vec{\varphi}_k). \qquad (5.7)\end{aligned}$$

This means that the convergence (in the large time steps limit) is to the state ρ' that is the solution of the following eigenvalue/integral equation with the largest eigenvalue (dominant eigenstate of $\mathcal{P}'$):

$$\int D\vec{\varphi}_k\,D\vec{\varphi}_{aux}\,P_{sub}(\vec{\varphi}_{k+1}|\vec{\varphi}_{aux})\,P_{sub}(\vec{\varphi}_{aux}|\vec{\varphi}_k)\,\rho'(\vec{\varphi}_k)=\rho'(\vec{\varphi}_{k+1}) \qquad (5.8)$$

Although this is off-course not the same as the original ground state (4.26) squared, this $\mathcal{P}'$ begins to produce an isotropic field configuration for increasing lattice discretization ε_x, but then saturates and doesn't get any better upon further increments. See simulation results (figures through 5.2 to 5.4). Clearly, the vertical correlator stays fairly consistent

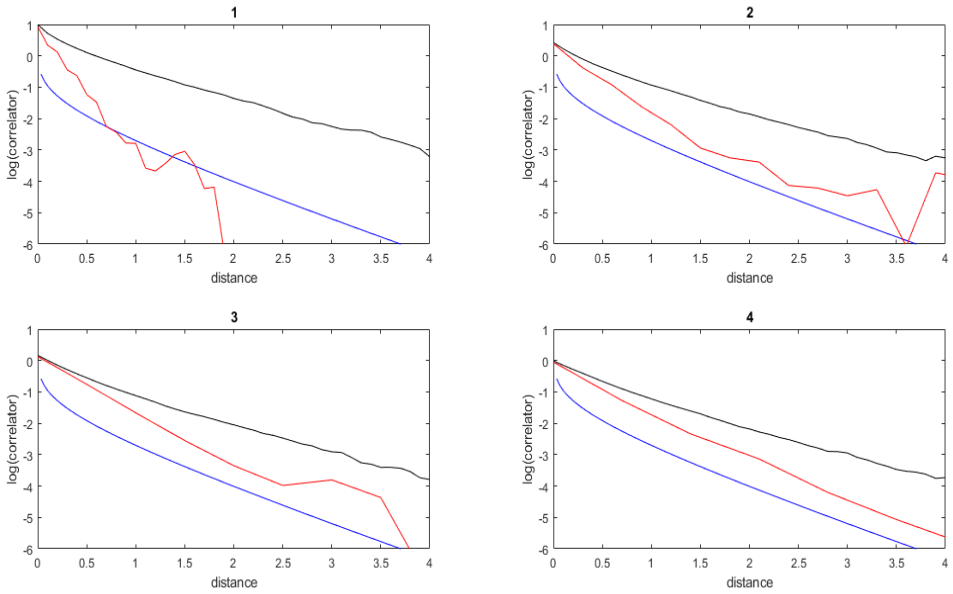

Figure 5.2: Graphs of $\log G_2(distance)$ vs *distance* for $m = 1$, $\varepsilon_t = 0.1/m$, with $\varepsilon_x/\varepsilon_t$ equal to $1, 3, 5$ and 7 respectively. Red and Black represent correlators along horizontal (space) and vertical (time) directions respectively, with blue being the theoretical one.

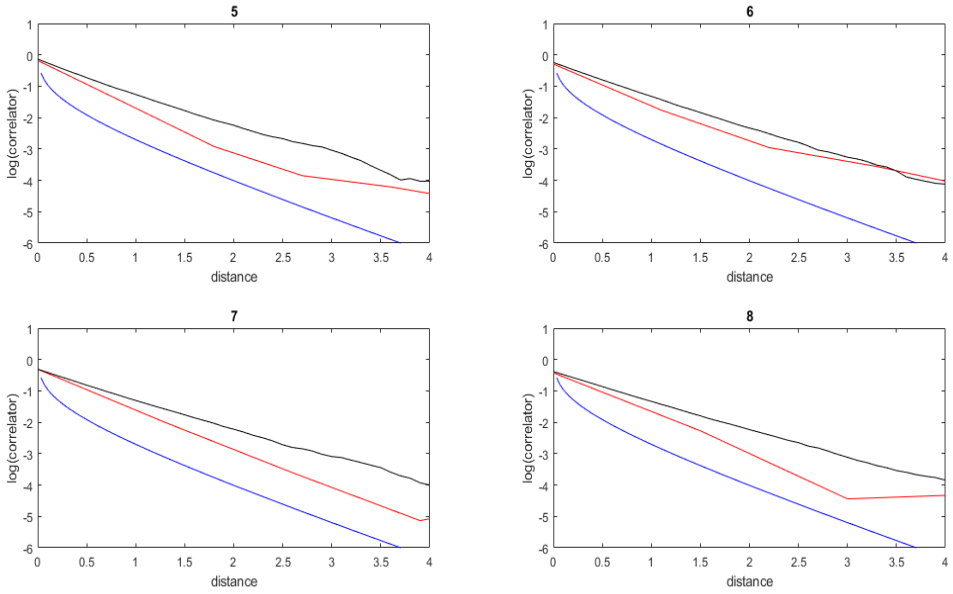

Figure 5.3: Graphs of $\log G_2(distance)$ vs *distance* for $m = 1$, $\varepsilon_t = 0.1/m$, with $\varepsilon_x/\varepsilon_t$ equal to $9, 11, 13$ and 15 respectively. Red and Black represent correlators along horizontal (space) and vertical (time) directions respectively, with blue being the theoretical one.

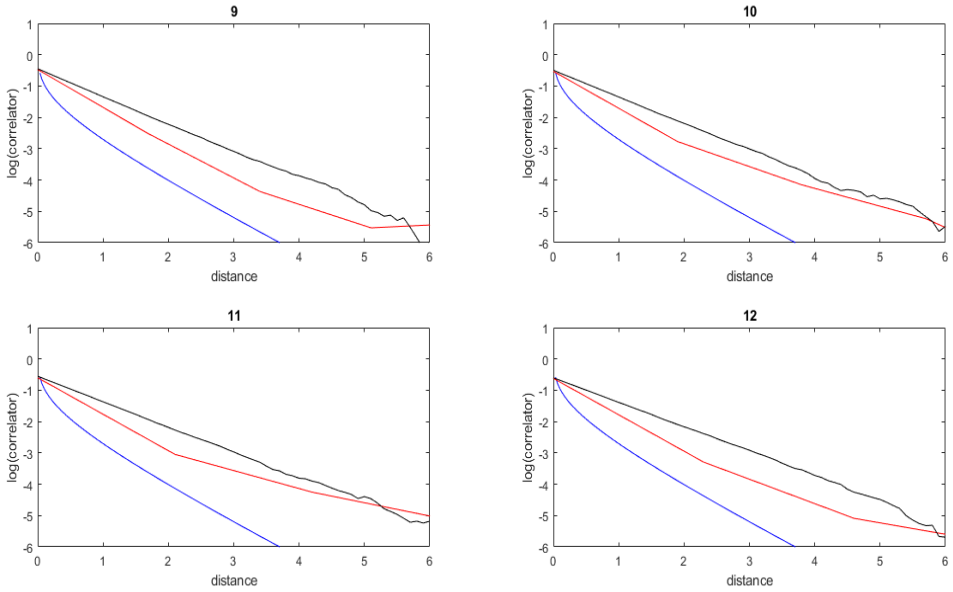

Figure 5.4: Graphs of $\log G_2(distance)$ vs $distance$ for $m = 1$, $\varepsilon_t = 0.1/m$, with $\varepsilon_x/\varepsilon_t$ equal to $17, 19, 21$ and 23 respectively. Red and Black represent correlators along horizontal (space) and vertical (time) directions respectively, with blue being the theoretical one.

and its only the horizontal correlator that shows variation. With increasing ε_x, the horizontal correlator seems to be getting closer to the vertical one, but then soon saturates around $\varepsilon_x \sim 1/m$, and is still far from the desired isotropy. Also, it fails to replicate the actual correlator (shown in blue), which is given by $K_0(md)$. Here, K_0 is the zeroth modified Bessel function of the second kind and d stands for the Euclidean distance between two points in a plane. Note however, that our main goal is to generate an isotropic field configuration first and then tune different parameters (perhaps by scanning the full parameter space, here $\varepsilon_x, \varepsilon_t$ and m) in the Markov processes which would replicate a given Lagrangian. Or stated otherwise: given that the isotropy is achieved, there must exist some Lagrangian which is represented by the network and the values of parameters used. In the present case, mimicking actual correlator was not guaranteed from the beginning itself, because there was a priori no reason as to why the block kernel (5.3), and hence p_{sub} should replicate the actual

$1+1$ Klein Gordon Lagrangian. I compare the numerical correlators with the actual one mainly for illustration purposes.

Now, one can try to impose some restrictions on the form of p_{sub} in order to ensure isotropy or maybe devise a whole new method to generate slices. Or maybe it is the case that such a checkerboard network does not produce desired isotropy at all, and that one needs more than just a 2-2 network, or needs to mix lattice sites differently, or both. These are some of the areas of current ongoing investigations.

6 Summary and Discussion

In this thesis report, I've addressed our goal of reducing the complexity of lattice simulation of homogeneous and isotropic Euclidean scalar fields. For the number of field values, space and time lattice sites being n, N_s^D and N respectively, the complexity is reduced from $(n^2)^{N_s^D N}$ to $N(n^2)^{N_s^D}$ where D is the number of spatial dimensions. That is, for $0+1$ fields there exists a simple and effective algorithm with linear complexity. This is done by simulating a typical field configuration point by point , using a Markov chain born out of the path integral (ground to ground state transition). For higher dimensional fields, a similar procedure may exist where a typical field configuration can be produced from 3 dimensional slices which still however, implies an exponential in space dependence as mentioned already (N_s^D to N_s^D Markov process). To reduce this exponential complexity (in space) for higher dimensional fields, I also discussed some potential techniques, namely Bayesian networks, and discussed a network in some detail.

I began by describing the basic physics involved in the introduction chapter where I over-viewed the Lagrangian formulation of classical and quantum mechanics and path integrals from the beginning, and finally transitioned to fields and their simulation on lattices. In the end, I've posed the mathematical statement of the problem. Then in chapter 2, I briefly described Markov chains and how they are used currently in Metropolis algorithm to simulate these fields. In chapter 3, I have discussed how the problem of simulating Gaussian fields reduces completely by going over to the diagonalized space (if off-course, the transformation is known) where at each lattice site there exists a normal Gaussian variable. The physical space field configuration is then obtained by inverse transforming back

to physical space. In chapter 4, I describe how a typical $D+1$ dimensional field configuration can be simulated through D dimensional slices via the Markov chain buried in the path integral for ground state to ground state transition. For quantum mechanics ($D=0$), slices are just points and we can easily simulate a typical $0+1$ field configuration point by point (time steps) since the Markov process (conditional probability distribution) is only a square matrix, the size of which depends on the number of field discretization points. I also present simulations for a harmonic and an-harmonic oscillator which match quite accurately with the free (harmonic) and small perturbation limit case. For higher dimensional ($D \geq 1$) fields and N_s lattice sites in each spatial direction, this Markov chain is still a high dimensional matrix (scaling exponentially $\sim N_s^D$). In chapter 5, I discuss some techniques involving Bayesian networks which can potentially reduce this exponentially complexity for higher dimensional fields further and is a potential direction to investigate further. I present a 2-2 network called checkerboard network along with its simulation results. Although this network is homogeneous by construction, the 2-2 Markov process I describe in this thesis begins to get isotropic with increasing spatial lattice discretization (with vertical behavior staying fairly consistent and horizontal getting closer to the former), but soon saturates around space discretization $\sim$ actual correlation length[1]. It therefore, fails to achieve the desired isotropy. This however does not mean that even the checkerboard network, let alone Bayesian networks in general, are proven to be non-working. There are yet many possible 2-2 Markov processes that need to be investigated in detail to see if there exists even just one, that can serve the purpose.

[1] for the Klein-Gordan case I considered, it is related to the only physical scale present in the problem i.e. $\sim 1/m$

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